Novel mononuclear and 1D-polymeric derivatives of lanthanides and (η^6-benzoic acid)tricarbonylchromium: Synthesis, structure and magnetic properties

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Supplementary materials

Table S1. Crystal data and structure refinement for **1, 2, 3a, 4a, 5a, Eu_1D, 3b, 4b, 5b, 6-9**.

Identification code	**1**	**2**	**3a**	**4a**	**5a**
Empirical formula	$C_{20}H_{23}CrEuO_{11}$	$C_{20}H_{23}CrGdO_{11}$	$C_{20}H_{23}CrO_{11}Tb$	$C_{20}H_{23}CrDyO_{11}$	$C_{20}H_{23}CrHoO_{11}$
Formula weight	643.34	648.63	650.30	653.88	656.32
Temperature, K	150(2)	150(2)	150(2)	150(2)	298
Wavelength, Å	0.71073	0.71073	0.71073	0.71073	1.5419
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic	Triclinic
Space group	P-1	P-1	P-1	P-1	P-1
a, Å	6.4895(2)	6.4819(5)	6.4691(3)	6.4695(2)	6.50560(2)
b, Å	13.6285(5)	13.6371(10)	13.6049(6)	13.5666(5)	13.6008(2)
c, Å	15.0080(5)	14.9951(11)	14.9858(7)	14.9597(5)	15.1041(3)
α, °	116.9370(10)	116.9023(19)	116.9850(10)	63.1180(10)	116.7781(15)
β, °	99.2120(10)	99.170(2)	99.0760(10)	79.2450(10)	99.444(3)
γ, °	91.9390(10)	91.939(2)	91.9810(10)	88.0100(10)	92.189(3)
Volume, $Å^3$	1159.51(7)	1158.45(15)	1152.13(9)	1148.70(7)	1167.36(6)
Z	2	2	2	2	2
D (calc), Mg/m^3	1.843	1.860	1.875	1.890	
μ, mm^{-1}	3.205	3.363	3.573	3.758	
F(000)	636	638	640	642	
Crystal size, mm	0.4 x 0.1 x 0.04	0.12 x 0.04 x 0.04	0.4 x 0.2 x 0.14	0.28 x 0.14 x 0.1	
θ range, °	2.761, 32.861	2.763, 27.786	2.764, 30.543	2.765, 32.861	
Index ranges	-9<=h<=9 -20<=k<=20 -22<=l<=22	-8<=h<=8 0<=k<=17 0<=l<=19	-9<=h<=9 -19<=k<=19 -21<=l<=21	-9<=h<=9 -20<=k<=19 -21<=l<=22	
Reflections collected	17561	5427	15965	17469	
Independent reflections, Rint	7891, 0.0350	5427, 0.0603	6885, 0.0295	7849, 0.0271	
Completeness to θ = 25.242°	99.9 %	99.9 %	99.9 %	99.9 %	
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	
Max,. min. transmission	0.7465, 0.5738	0.7456, 0.5664	0.7461, 0.4892	0.7465, 0.4979	
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	

Data / restraints / parameters	7891 / 0 / 302	5427 / 0 / 302	6885 / 0 / 317	7849 / 0 / 302
Goodness-of-fit	1.008	1.091	0.858	1.045
R1, wR2 [I>2sigma(I)]	0.0335, 0.0706	0.0461, 0.1045	0.0246, 0.0631	0.0263, 0.0626
R1, wR2 (all data)	0.0405, 0.0735	0.0652, 0.1141	0.0297, 0.0660	0.0308, 0.0643
Largest diff. peak and hole, e.Å^{-3}	1.961, -1.737	3.039, -1.603	1.536, -0.779	2.170, -1.093

Identification code	**Eu_1D**	**4b**	**5b**	**8**
Empirical formula	$C_{20}H_{21}CrEuO_{10}$	$C_{20}H_{21}CrDyO_{10}$	$C_{20}H_{21}CrHoO_{10}$	$C_{20}H_{21}CrO_{10}Yb$
Formula weight	625.33	635.87	638.30	646.41
Temperature, K	150(2)	150(2)	150(2)	150(2)
Wavelength, Å	0.71073	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	C2/c	C2/c	C2/c	C2/c
a, Å	23.3696(10)	23.2279(7)	23.2334(8)	23.0974(9)
b, Å	10.6048(5)	10.5289(3)	10.5294(4)	10.4746(4)
c, Å	18.9372(8)	18.9114(5)	18.9043(6)	18.9178(7)
β, °	94.2180(10)	94.0750(10)	94.0130(10)	93.9870(10)
Volume, Å^3	4680.5(4)	4613.4(2)	4613.3(3)	4565.8(3)
Z	8	8	8	8
D (calc), Mg/m^3	1.775	1.831	1.838	1.881
μ, mm^{-1}	3.170	3.737	3.927	4.599
F(000)	2464	2488	2496	2520
Crystal size, mm	0.24 x 0.12 x 0.1	0.15 x 0.03 x 0.03	0.28 x 0.2 x 0.12	0.16 x 0.08 x 0.06
θ range, °	2.340, 30.051	2.355, 28.306	2.355, 33.148	2.365, 30.058
Index ranges	-32<=h<=32	-30<=h<=30	-35<=h<=35	-32<=h<=32
	-14<=k<=14	-14<=k<=14	-15<=k<=16	-14<=k<=14
	-26<=l<=26	-24<=l<=25	-29<=l<=28	-26<=l<=26
Reflections collected	31667	27720	47696	30982
Independent reflections, Rint	6845, 0.0494	5701, 0.0724	8510, 0.0336	6684, 0.0626
Completeness to θ = 25.242°	99.9 %	99.9 %	99.9 %	99.9 %
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
Max,. min. transmission	0.746, 0.5556	0.7457, 0.5928	0.7465, 0.5209	0.746, 0.5843

Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	6845 / 0 / 299	5701 / 0 / 289	8510 / 0 / 299	6684 / 0 / 299
Goodness-of-fit	0.966	0.926	1.112	0.971
R1, wR2 [I>2sigma(I)]	0.0264, 0.0559	0.0334, 0.0602	0.0209, 0.0422	0.0309, 0.0615
R1, wR2 (all data)	0.0445, 0.0614	0.0591, 0.0674	0.0311, 0.0452	0.0493, 0.0678
Largest diff. peak and hole, e.Å^{-3}	1.327, -0.609	0.896, -0.645	1.061, -0.811	1.080, -0.909
Identification code	**3b**	**6**	**7**	**9**
Empirical formula	$C_{20}H_{21}CrO_{10}Tb$	$C_{20}H_{21}CrErO_{10}$	$C_{20}H_{21}CrO_{10}Tm$	$C_{20}H_{21}CrO_{10}Y$
Formula weight	632.30	640.63	642.31	562.28
Temperature, K	298	298	298	298
Wavelength, Å	1.5419	1.5419	1.5419	1.5419
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	C2/c	C2/c	C2/c	C2/c
a, Å	23.4054(13)	23.3571(6)	23.3040(7)	23.3760(10)
b, Å	10.6144(10)	10.5742(3)	10.5547(6)	10.5560(17)
c, Å	18.9095(16)	18.9852(5)	18.96240(7)	18.9751(8)
β, °	93.845(6)	93.694(2)	93.716(3)	93.815(9)
Volume, Å^3	4687.2(6)	4679.3(2)	4654.3(3)	4671.9(8)
Z	8	8	8	8

Table S2. Crystal data and Rietveld refinement for **5a, 3b, 6, 7, 9**.

5a

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File                                        1                                        :
D:\Andr\Paper\Gavrikov2\Powder\Ho_Gav061\Ho_acac_Cr_CO_Ph_COO_2015_08_18.raw_1
Range Number :  1

Number of independent parameters : 22

R-Values

Rexp : 2.87    Rwp : 7.76     Rp  : 5.59   GOF : 2.70
Rexp`: 6.53    Rwp`: 17.65    Rp` : 17.66  DW  : 0.41

Quantitative Analysis - Rietveld
   Phase 1  : [HoCrCOO(acac)2(H2O)2]       100.000 %

Background
   Chebychev polynomial, Coefficient  0      826.9(16)
                                      1      -42.1(24)
                                      2      -29.6(23)
                                      3      38.3(22)
                                      4      -53.0(20)
                                      5      1.7(20)
                                      6      30.4(18)
                                      7      -33.9(19)

Instrument
   Primary radius (mm)                      280
   Secondary radius (mm)                    280
   Full Axial Convolution
      Filament length (mm)                  12
      Sample length (mm)                    12
      Receiving Slit length (mm)            12
      Primary Sollers (°)                   2.5
      Secondary Sollers (°)                 2.5

Corrections
   Specimen displacement                    -0.3422346
   LP Factor                                0

Miscellaneous
   Start X                                  4
   Finish X                                 60

Structure 1
   Phase name                               [HoCrCOO(acac)2(H2O)2]
   R-Bragg                                  5.067
   Spacegroup                               P-1
   Scale                                    0.00013830(61)
   Cell Mass                                1312.649
   Cell Volume (A^3)                        1167.356(58)
   Wt% - Rietveld                           100.000
   Crystal Linear Absorption Coeff. (1/cm)  104.3712(52)
   Crystal Density (g/cm^3)                 1.867217(92)
   Preferred Orientation (Dir 1 : 1 0 0)    1.627(11)
                         (Dir 2 : 0 1 1)    0.5871(49)
      Fraction of Dir 1                     0.649(10)
   PV_TCHZ peak type
      U                                     0.0024(45)
      V                                     0.0069(15)
      W                                     0.000420(92)
      Z                                     0
      X                                     0.0938(34)
      Y                                     0
   Lattice parameters
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a (A)	6.50559(24)
b (A)	13.60081(24)
c (A)	15.10409(26)
alpha (°)	116.7781(15)
beta (°)	99.4445(30)
gamma (°)	92.1890(34)

Site	Np	x	y	z	Atom	Occ	Beq
Ho1	2	0.23387	0.47926	0.17210	Ho	1	2
Cr1	2	0.06491	0.22257	0.39046	Cr	1	2
O1	2	0.32350	0.46250	0.32901	O	1	3
O2	2	-0.01140	0.41605	0.24950	O	1	3
O3	2	-0.03470	0.35695	0.03160	O	1	3
O4	2	0.33470	0.30192	0.11475	O	1	3
O5	2	-0.02900	0.59967	0.17835	O	1	3
O6	2	0.37900	0.66282	0.29172	O	1	3
O7	2	0.29340	0.52510	0.03642	O	1	3
H1	2	0.21500	0.57110	0.02180	H	1	4
H2A	2	0.42540	0.51850	0.02500	H	0.5	4
H2B	2	0.24390	0.46600	-0.02450	H	0.5	4
O8	2	0.61060	0.48109	0.17779	O	1	3
H3	2	0.70840	0.44920	0.20190	H	1	4
H4	2	0.70290	0.52730	0.17150	H	1	4
O9	2	0.44090	0.10410	0.33210	O	1	3
O10	2	-0.13810	0.09050	0.16980	O	1	3
O11	2	-0.09910	0.02920	0.41440	O	1	3
C1	2	0.13660	0.42380	0.32020	C	1	3
C2	2	0.08780	0.38840	0.39650	C	1	3
C3	2	0.25450	0.38810	0.46930	C	1	3
H3A	2	0.39530	0.40740	0.46760	H	1	4
C4	2	0.21420	0.35940	0.54450	C	1	3
H4A	2	0.32650	0.36100	0.59450	H	1	4
C5	2	0.00570	0.32830	0.54460	C	1	3
H5A	2	-0.02250	0.30700	0.59400	H	1	4
C6	2	-0.16190	0.32850	0.47240	C	1	3
H6A	2	-0.30240	0.30920	0.47450	H	1	4
C7	2	-0.12220	0.35700	0.39770	C	1	3
H7A	2	-0.23520	0.35530	0.34800	H	1	4
C8	2	-0.31220	0.21090	-0.06460	C	1	3
H8A	2	-0.33740	0.13040	-0.09110	H	1	3
H8B	2	-0.32880	0.22860	-0.12160	H	1	3
H8C	2	-0.41350	0.24650	-0.02140	H	1	3
C9	2	-0.09280	0.25250	-0.00280	C	1	3
C10	2	0.03040	0.17860	0.01310	C	1	3
H10A	2	-0.02970	0.10350	-0.01690	H	1	4
C11	2	0.23600	0.20560	0.06980	C	1	3
C12	2	0.35150	0.11600	0.07960	C	1	3
H12A	2	0.29300	0.04400	0.02150	H	1	4
H12B	2	0.33570	0.11500	0.14310	H	1	4
H12C	2	0.50090	0.13060	0.08060	H	1	4
C13	2	-0.22860	0.74240	0.17960	C	1	3
H13A	2	-0.22450	0.82270	0.22120	H	1	4
H13B	2	-0.35050	0.70430	0.18700	H	1	4
H13C	2	-0.23980	0.72480	0.10790	H	1	4
C14	2	-0.03150	0.70510	0.21440	C	1	3
C15	2	0.13460	0.78350	0.28220	C	1	3
H15A	2	0.11560	0.85940	0.30520	H	1	4
C16	2	0.32940	0.75950	0.31960	C	1	3
C17	2	0.48680	0.85550	0.39850	C	1	3
H17A	2	0.48830	0.91580	0.38000	H	1	4
H17B	2	0.62700	0.83120	0.40170	H	1	4
H17C	2	0.44740	0.88180	0.46530	H	1	4
C18	2	0.29930	0.15220	0.35600	C	1	3
C19	2	-0.06020	0.14300	0.25420	C	1	3
C20	2	-0.03400	0.10370	0.40560	C	1	3

3a

File 1 : D:\Andr\Paper\Gavrikov2\Powder\Tb\Tb_Cr_2016_03_16.raw_1
Range Number : 1

Number of independent parameters : 19

R-Values

Rexp : 2.99	Rwp : 6.12	Rp : 4.32	GOF : 2.05
Rexp`: 11.19	Rwp`: 22.93	Rp` : 22.20	DW : 0.75

Quantitative Analysis - Rietveld

Phase 1 : TbrCrCOO(acac)2(H2O)]n		100.000 %

Background

One on X		1800(2100)
Chebychev polynomial, Coefficient	0	870(120)
	1	160(130)
	2	-91(73)
	3	27(40)
	4	22(22)
	5	-32(12)
	6	29.7(61)
	7	1.8(38)

Instrument

Primary radius (mm)	280
Secondary radius (mm)	280
Full Axial Convolution	
Filament length (mm)	12
Sample length (mm)	15
Receiving Slit length (mm)	12
Primary Sollers (°)	2.5
Secondary Sollers (°)	2.5

Corrections

Specimen displacement	-0.6375525
LP Factor	0

Miscellaneous

Start X	5
Finish X	60

Structure 1

Phase name	TbrCrCOO(acac)2(H2O)]n
R-Bragg	3.576
Spacegroup	C2/c
Scale	0.000002924(35)
Cell Mass	5058.416
Cell Volume (A^3)	4687.19(63)
Wt% - Rietveld	100.000
Crystal Linear Absorption Coeff. (1/cm)	183.911(25)
Crystal Density (g/cm^3)	1.79205(24)
Preferred Orientation (Dir 1 : 1 0 0)	0.8629(32)
PV_TCHZ peak type	
U	0.584(52)
V	-0.230(15)
W	0.0253(10)
Z	0
X	0.096(19)
Y	0
Lattice parameters	
a (A)	23.4054(13)

b (A)		10.61442(96)
c (A)		18.9095(16)
beta (°)		93.8446(58)

Site	Np	x	y	z	Atom	Occ	Beq
Tb1	8	0.25197	0.59172	0.23468	Tb	1	2
Cr1	8	0.39416	0.27818	0.04433	Cr	1	3
O1	8	0.27403	0.44319	0.15424	O	1	3
O2	8	0.27261	0.24213	0.18972	O	1	3
O3	8	0.32503	0.72206	0.20033	O	1	3
O4	8	0.33697	0.52498	0.29597	O	1	3
O5	8	0.21228	0.70990	0.14205	O	1	3
O6	8	0.15707	0.52553	0.21699	O	1	3
O7	8	0.45077	0.53471	0.05704	O	1	3
O8	8	0.50161	0.17490	-0.01397	O	1	3
O9	8	0.44356	0.21616	0.19119	O	1	3
O10	8	0.23262	0.44182	0.32284	O	1	3
H1	8	0.26390	0.39050	0.33900	H	1	4
H2	8	0.20730	0.38770	0.31210	H	1	4
C1	8	0.28262	0.32710	0.14549	C	1	3
C2	8	0.30467	0.28633	0.07660	C	1	3
C3	8	0.31120	0.37613	0.02269	C	1	3
H3A	8	0.30200	0.46270	0.03050	H	1	4
C4	8	0.33136	0.33871	-0.04334	C	1	3
H4A	8	0.33480	0.39920	-0.08010	H	1	4
C5	8	0.34610	0.21120	-0.05369	C	1	3
H5A	8	0.36050	0.18580	-0.09730	H	1	4
C6	8	0.33969	0.12022	0.00002	C	1	3
H6A	8	0.34910	0.03380	-0.00790	H	1	4
C7	8	0.31957	0.15710	0.06472	C	1	3
H7A	8	0.31580	0.09590	0.10100	H	1	4
C8	8	0.40876	0.80320	0.15232	C	1	3
H8A	8	0.40150	0.88960	0.16870	H	1	4
H8B	8	0.39350	0.79410	0.10290	H	1	4
H8C	8	0.45040	0.78700	0.15560	H	1	4
C9	8	0.37945	0.70941	0.19789	C	1	3
C10	8	0.41179	0.61725	0.23511	C	1	3
H10A	8	0.45160	0.61090	0.22700	H	1	4
C11	8	0.38988	0.53309	0.28371	C	1	3
C12	8	0.43095	0.44750	0.32672	C	1	3
H12A	8	0.41790	0.35930	0.32160	H	1	4
H12B	8	0.43190	0.47220	0.37680	H	1	4
H12C	8	0.46970	0.45540	0.30970	H	1	4
C13	8	0.16389	0.79030	0.03781	C	1	3
H13A	8	0.12480	0.78980	0.01460	H	1	4
H13B	8	0.19130	0.76040	0.00440	H	1	4
H13C	8	0.17410	0.87690	0.05300	H	1	4
C14	8	0.16609	0.70437	0.10129	C	1	4
C15	8	0.11898	0.62720	0.11271	C	1	4
H15A	8	0.08670	0.63060	0.07910	H	1	4
C16	8	0.11618	0.54520	0.17039	C	1	3
C17	8	0.06023	0.47530	0.17918	C	1	3
H17A	8	0.06830	0.38500	0.18770	H	1	4
H17B	8	0.03470	0.48470	0.13600	H	1	4
H17C	8	0.04140	0.51090	0.21950	H	1	4
C18	8	0.42927	0.43617	0.05227	C	1	3
C19	8	0.46061	0.21560	0.00835	C	1	3
C20	8	0.42477	0.23990	0.13524	C	1	3

6

File 1 :
D:\Andr\Paper\Gavrikov2\Powder\Er_Gav071\Er_acac_Cr_CO_Ph_COO_2015_07_28_sysh
.raw_1
Range Number : 1

Number of independent parameters : 21

R-Values

Rexp : 3.93 Rwp : 6.09 Rp : 4.83 GOF : 1.55
Rexp`: 4.06 Rwp`: 6.29 Rp` : 5.76 DW : 0.94

Quantitative Analysis - Rietveld
Phase 1 : Structure 100.000 %

Background

One on X		5170(410)
Chebychev polynomial, Coefficient	0	4(33)
	1	450(40)
	2	-284(24)
	3	175(15)
	4	-88.6(85)
	5	20.9(52)
	6	5.1(29)
	7	-3.0(20)

Instrument

Primary radius (mm)	280
Secondary radius (mm)	280
Full Axial Convolution	
Filament length (mm)	12
Sample length (mm)	15
Receiving Slit length (mm)	12
Primary Sollers (°)	2.5
Secondary Sollers (°)	2.5

Corrections

Specimen displacement	-0.3317539
LP Factor	0

Structure 1

Phase name	Structure
R-Bragg	3.630
Spacegroup	C2/c
Scale	0.000004569(20)
Cell Mass	5125.112
Cell Volume (A^3)	4679.28(22)
Wt% - Rietveld	100.000
Crystal Linear Absorption Coeff. (1/cm)	107.2943(50)
Crystal Density (g/cm^3)	1.818753(85)
Preferred Orientation (Dir 1 : 1 1 0)	1.294(51)
(Dir 2 : 0 0 1)	0.9816(66)
Fraction of Dir 1	0.425(61)
PV_TCHZ peak type	
U	-0.138(16)
V	0.0375(52)
W	0.00005(30)
Z	0
X	0.1700(52)
Y	0
Lattice parameters	
a (A)	23.35713(55)

b (A)		10.57420(34)
c (A)		18.98521(46)
beta (°)		93.6937(23)

Site	Np	x	y	z	Atom	Occ	Beq
Er1	8	0.25197	0.59172	0.23468	Er	1	2
Cr1	8	0.39416	0.27818	0.04433	Cr	1	3
O1	8	0.27403	0.44319	0.15424	O	1	3
O2	8	0.27261	0.24213	0.18972	O	1	3
O3	8	0.32503	0.72206	0.20033	O	1	3
O4	8	0.33697	0.52498	0.29597	O	1	3
O5	8	0.21228	0.70990	0.14205	O	1	3
O6	8	0.15707	0.52553	0.21699	O	1	3
O7	8	0.45077	0.53471	0.05704	O	1	3
O8	8	0.50161	0.17490	-0.01397	O	1	3
O9	8	0.44356	0.21616	0.19119	O	1	3
O10	8	0.23262	0.44182	0.32284	O	1	3
H1	8	0.26390	0.39050	0.33900	H	1	4
H2	8	0.20730	0.38770	0.31210	H	1	4
C1	8	0.28262	0.32710	0.14549	C	1	3
C2	8	0.30467	0.28633	0.07660	C	1	3
C3	8	0.31120	0.37613	0.02269	C	1	3
H3A	8	0.30200	0.46270	0.03050	H	1	4
C4	8	0.33136	0.33871	-0.04334	C	1	3
H4A	8	0.33480	0.39920	-0.08010	H	1	4
C5	8	0.34610	0.21120	-0.05369	C	1	3
H5A	8	0.36050	0.18580	-0.09730	H	1	4
C6	8	0.33969	0.12022	0.00002	C	1	3
H6A	8	0.34910	0.03380	-0.00790	H	1	4
C7	8	0.31957	0.15710	0.06472	C	1	3
H7A	8	0.31580	0.09590	0.10100	H	1	4
C8	8	0.40876	0.80320	0.15232	C	1	3
H8A	8	0.40150	0.88960	0.16870	H	1	4
H8B	8	0.39350	0.79410	0.10290	H	1	4
H8C	8	0.45040	0.78700	0.15560	H	1	4
C9	8	0.37945	0.70941	0.19789	C	1	3
C10	8	0.41179	0.61725	0.23511	C	1	3
H10A	8	0.45160	0.61090	0.22700	H	1	4
C11	8	0.38988	0.53309	0.28371	C	1	3
C12	8	0.43095	0.44750	0.32672	C	1	3
H12A	8	0.41790	0.35930	0.32160	H	1	4
H12B	8	0.43190	0.47220	0.37680	H	1	4
H12C	8	0.46970	0.45540	0.30970	H	1	4
C13	8	0.16389	0.79030	0.03781	C	1	3
H13A	8	0.12480	0.78980	0.01460	H	1	4
H13B	8	0.19130	0.76040	0.00440	H	1	4
H13C	8	0.17410	0.87690	0.05300	H	1	4
C14	8	0.16609	0.70437	0.10129	C	1	4
C15	8	0.11898	0.62720	0.11271	C	1	4
H15A	8	0.08670	0.63060	0.07910	H	1	4
C16	8	0.11618	0.54520	0.17039	C	1	3
C17	8	0.06023	0.47530	0.17918	C	1	3
H17A	8	0.06830	0.38500	0.18770	H	1	4
H17B	8	0.03470	0.48470	0.13600	H	1	4
H17C	8	0.04140	0.51090	0.21950	H	1	4
C18	8	0.42927	0.43617	0.05227	C	1	3
C19	8	0.46061	0.21560	0.00835	C	1	3
C20	8	0.42477	0.23990	0.13524	C	1	3

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Range Number : 1

Number of independent parameters : 20

R-Values

Rexp : 2.93	Rwp : 8.69	Rp : 6.48	GOF : 2.97
Rexp`: 6.46	Rwp`: 19.17	Rp` : 19.05	DW : 0.49

Quantitative Analysis - Rietveld
Phase 1 : [TmCrCOO(acac)2(H2O)]n 100.000 %

Background

Chebychev polynomial, Coefficient	0	776.2(28)
	1	-42.6(42)
	2	-10.8(39)
	3	-31.3(38)
	4	56.5(35)
	5	-30.5(35)
	6	0.9(31)
	7	31.4(31)

Instrument

Primary radius (mm)	280
Secondary radius (mm)	280
Full Axial Convolution	
Filament length (mm)	12
Sample length (mm)	15
Receiving Slit length (mm)	12
Primary Sollers (°)	2.5
Secondary Sollers (°)	2.5

Corrections

Specimen displacement	-0.5809385
LP Factor	0

Miscellaneous

Start X	4
Finish X	50

Structure 1

Phase name	[TmCrCOO(acac)2(H2O)]n
R-Bragg	6.495
Spacegroup	C2/c
Scale	0.000006123(47)
Cell Mass	5138.506
Cell Volume (A^3)	4654.30(34)
Wt% - Rietveld	100.000
Crystallite Size	
Cry size Gaussian (nm)	150.0
Crystal Linear Absorption Coeff. (1/cm)	111.7363(82)
Crystal Density (g/cm^3)	1.83329(13)
Preferred Orientation (Dir 1 : 1 0 0)	0.724(34)
(Dir 2 : 0 1 0)	1.267(14)
Fraction of Dir 1	0.208(44)
PV_TCHZ peak type	
U	0.001(10)
V	-0.0157(36)
W	0.00348(27)
Z	0
X	0.0428(65)

Y 0

Lattice parameters

a (A) 23.30396(68)

b (A) 10.55469(59)

c (A) 18.96239(70)

beta (°) 93.7160(31)

Site	Np	x	y	z	Atom	Occ	Beq
Tm1	8	0.25197	0.59172	0.23468	Tm	1	1
Cr1	8	0.39416	0.27818	0.04433	Cr	1	2
O1	8	0.27403	0.44319	0.15424	O	1	2
O2	8	0.27261	0.24213	0.18972	O	1	2
O3	8	0.32503	0.72206	0.20033	O	1	2
O4	8	0.33697	0.52498	0.29597	O	1	2
O5	8	0.21228	0.70990	0.14205	O	1	2
O6	8	0.15707	0.52553	0.21699	O	1	2
O7	8	0.45077	0.53471	0.05704	O	1	2
O8	8	0.50161	0.17490	-0.01397	O	1	2
O9	8	0.44356	0.21616	0.19119	O	1	2
O10	8	0.23262	0.44182	0.32284	O	1	2
H1	8	0.26390	0.39050	0.33900	H	1	4
H2	8	0.20730	0.38770	0.31210	H	1	4
C1	8	0.28262	0.32710	0.14549	C	1	3
C2	8	0.30467	0.28633	0.07660	C	1	3
C3	8	0.31120	0.37613	0.02269	C	1	3
H3A	8	0.30200	0.46270	0.03050	H	1	4
C4	8	0.33136	0.33871	-0.04334	C	1	3
H4A	8	0.33480	0.39920	-0.08010	H	1	4
C5	8	0.34610	0.21120	-0.05369	C	1	3
H5A	8	0.36050	0.18580	-0.09730	H	1	4
C6	8	0.33969	0.12022	0.00002	C	1	3
H6A	8	0.34910	0.03380	-0.00790	H	1	4
C7	8	0.31957	0.15710	0.06472	C	1	3
H7A	8	0.31580	0.09590	0.10100	H	1	4
C8	8	0.40876	0.80320	0.15232	C	1	3
H8A	8	0.40150	0.88960	0.16870	H	1	4
H8B	8	0.39350	0.79410	0.10290	H	1	4
H8C	8	0.45040	0.78700	0.15560	H	1	4
C9	8	0.37945	0.70941	0.19789	C	1	3
C10	8	0.41179	0.61725	0.23511	C	1	3
H10A	8	0.45160	0.61090	0.22700	H	1	4
C11	8	0.38988	0.53309	0.28371	C	1	3
C12	8	0.43095	0.44750	0.32672	C	1	3
H12A	8	0.41790	0.35930	0.32160	H	1	4
H12B	8	0.43190	0.47220	0.37680	H	1	4
H12C	8	0.46970	0.45540	0.30970	H	1	4
C13	8	0.16389	0.79030	0.03781	C	1	3
H13A	8	0.12480	0.78980	0.01460	H	1	4
H13B	8	0.19130	0.76040	0.00440	H	1	4
H13C	8	0.17410	0.87690	0.05300	H	1	4
C14	8	0.16609	0.70437	0.10129	C	1	3
C15	8	0.11898	0.62720	0.11271	C	1	3
H15A	8	0.08670	0.63060	0.07910	H	1	4
C16	8	0.11618	0.54520	0.17039	C	1	3
C17	8	0.06023	0.47530	0.17918	C	1	3
H17A	8	0.06830	0.38500	0.18770	H	1	4
H17B	8	0.03470	0.48470	0.13600	H	1	4
H17C	8	0.04140	0.51090	0.21950	H	1	4
C18	8	0.42927	0.43617	0.05227	C	1	3
C19	8	0.46061	0.21560	0.00835	C	1	3
C20	8	0.42477	0.23990	0.13524	C	1	3

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Range Number : 1

Number of independent parameters : 22

R-Values

Rexp : 4.53	Rwp : 8.61	Rp : 6.06	GOF : 1.90
Rexp`: 12.52	Rwp`: 23.79	Rp` : 19.24	DW : 0.92

Quantitative Analysis - Rietveld

Phase 1 : Structure	100.000 %

Background

One on X		1800(2500)
Chebychev polynomial, Coefficient	0	440(180)
	1	-340(200)
	2	290(110)
	3	-159(60)
	4	105(33)
	5	-109(18)
	6	101.9(98)
	7	-63.4(47)
	8	25.0(25)

Instrument

Primary radius (mm)	280
Secondary radius (mm)	280
Full Axial Convolution	
Filament length (mm)	12
Sample length (mm)	8
Receiving Slit length (mm)	12
Primary Sollers (°)	2.5
Secondary Sollers (°)	2.5

Corrections

Specimen displacement	-0.09
LP Factor	0

Miscellaneous

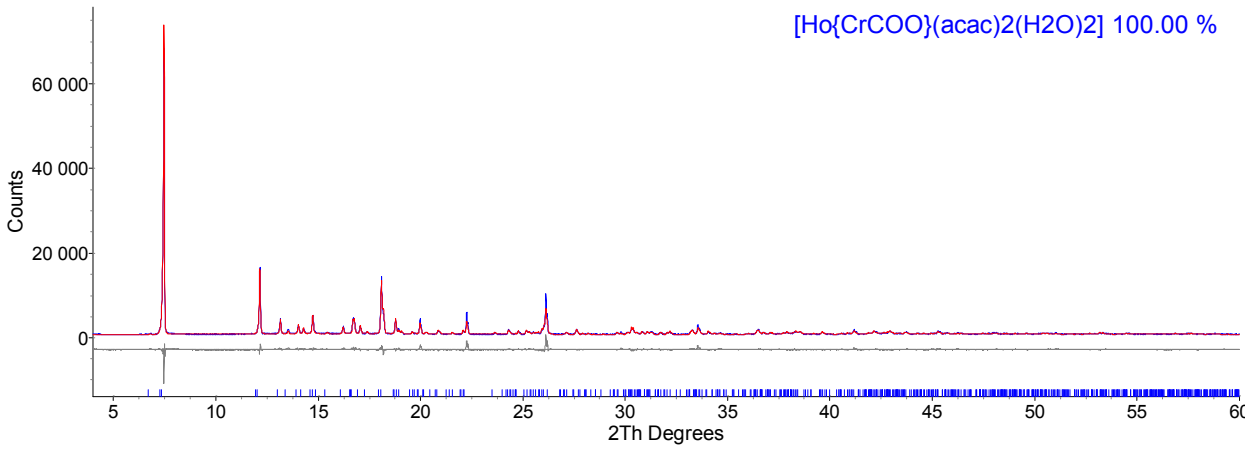
Start X	4
Finish X	50

Structure 1

Phase name	Structure
R-Bragg	5.709
Spacegroup	C2/c
Scale	0.000001306(25)
Cell Mass	4498.264
Cell Volume (A^3)	4671.86(79)
Wt% - Rietveld	100.000
Crystal Linear Absorption Coeff. (1/cm)	76.556(13)
Crystal Density (g/cm^3)	1.59884(27)
Preferred Orientation (Dir 1 : 1 0 0)	0.6044(89)
(Dir 2 : 0 0 1)	0.3573(68)
Fraction of Dir 1	0.572(23)
PV_TCHZ peak type	
U	0.119(25)
V	-0.0179(40)
W	0.00067(22)
Z	0

X	0.101(17)
Y	0
Lattice parameters	
a (A)	23.3760(10)
b (A)	10.5560(17)
c (A)	18.97507(80)
beta (°)	93.8148(88)

Site	Np	x	y	z	Atom	Occ	Beq
Y1	8	0.25197	0.59172	0.23468	Y	1	4
Cr1	8	0.39416	0.27818	0.04433	Cr	1	4
O1	8	0.27403	0.44319	0.15424	O	1	4
O2	8	0.27261	0.24213	0.18972	O	1	4
O3	8	0.32503	0.72206	0.20033	O	1	4
O4	8	0.33697	0.52498	0.29597	O	1	4
O5	8	0.21228	0.70990	0.14205	O	1	4
O6	8	0.15707	0.52553	0.21699	O	1	4
O7	8	0.45077	0.53471	0.05704	O	1	4
O8	8	0.50161	0.17490	-0.01397	O	1	4
O9	8	0.44356	0.21616	0.19119	O	1	4
O10	8	0.23262	0.44182	0.32284	O	1	4
H1	8	0.26390	0.39050	0.33900	H	1	6
H2	8	0.20730	0.38770	0.31210	H	1	6
C1	8	0.28262	0.32710	0.14549	C	1	4
C2	8	0.30467	0.28633	0.07660	C	1	4
C3	8	0.31120	0.37613	0.02269	C	1	4
H3A	8	0.30200	0.46270	0.03050	H	1	6
C4	8	0.33136	0.33871	-0.04334	C	1	4
H4A	8	0.33480	0.39920	-0.08010	H	1	6
C5	8	0.34610	0.21120	-0.05369	C	1	4
H5A	8	0.36050	0.18580	-0.09730	H	1	6
C6	8	0.33969	0.12022	0.00002	C	1	4
H6A	8	0.34910	0.03380	-0.00790	H	1	6
C7	8	0.31957	0.15710	0.06472	C	1	4
H7A	8	0.31580	0.09590	0.10100	H	1	6
C8	8	0.40876	0.80320	0.15232	C	1	4
H8A	8	0.40150	0.88960	0.16870	H	1	6
H8B	8	0.39350	0.79410	0.10290	H	1	6
H8C	8	0.45040	0.78700	0.15560	H	1	6
C9	8	0.37945	0.70941	0.19789	C	1	4
C10	8	0.41179	0.61725	0.23511	C	1	4
H10A	8	0.45160	0.61090	0.22700	H	1	6
C11	8	0.38988	0.53309	0.28371	C	1	4
C12	8	0.43095	0.44750	0.32672	C	1	4
H12A	8	0.41790	0.35930	0.32160	H	1	6
H12B	8	0.43190	0.47220	0.37680	H	1	6
H12C	8	0.46970	0.45540	0.30970	H	1	6
C13	8	0.16389	0.79030	0.03781	C	1	4
H13A	8	0.12480	0.78980	0.01460	H	1	6
H13B	8	0.19130	0.76040	0.00440	H	1	6
H13C	8	0.17410	0.87690	0.05300	H	1	6
C14	8	0.16609	0.70437	0.10129	C	1	4
C15	8	0.11898	0.62720	0.11271	C	1	4
H15A	8	0.08670	0.63060	0.07910	H	1	6
C16	8	0.11618	0.54520	0.17039	C	1	4
C17	8	0.06023	0.47530	0.17918	C	1	4
H17A	8	0.06830	0.38500	0.18770	H	1	6
H17B	8	0.03470	0.48470	0.13600	H	1	6
H17C	8	0.04140	0.51090	0.21950	H	1	6
C18	8	0.42927	0.43617	0.05227	C	1	4
C19	8	0.46061	0.21560	0.00835	C	1	4
C20	8	0.42477	0.23990	0.13524	C	1	4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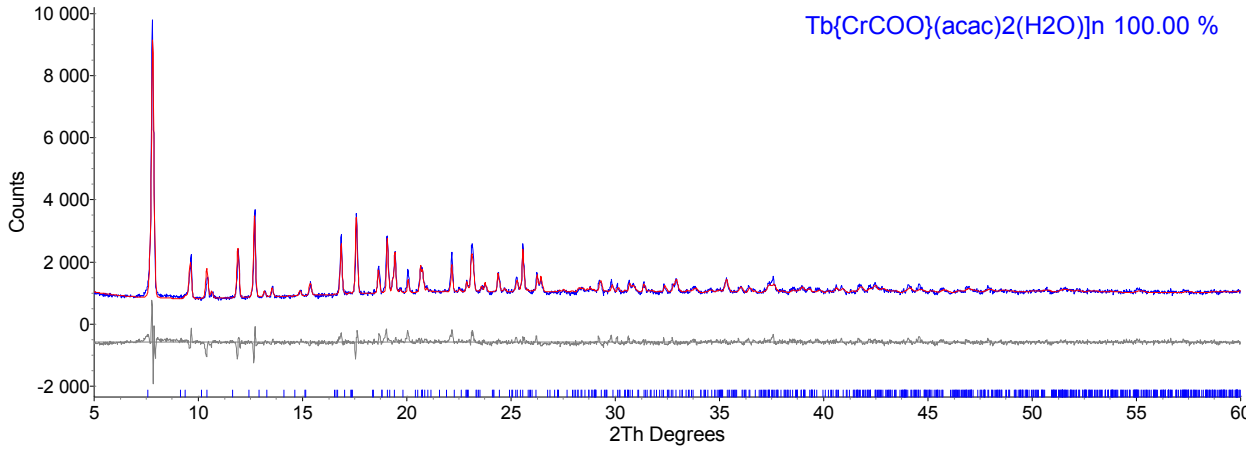
20 000
0
5
10
15
20
25
30
35
40
45
50
55
2Th Degrees

a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Counts
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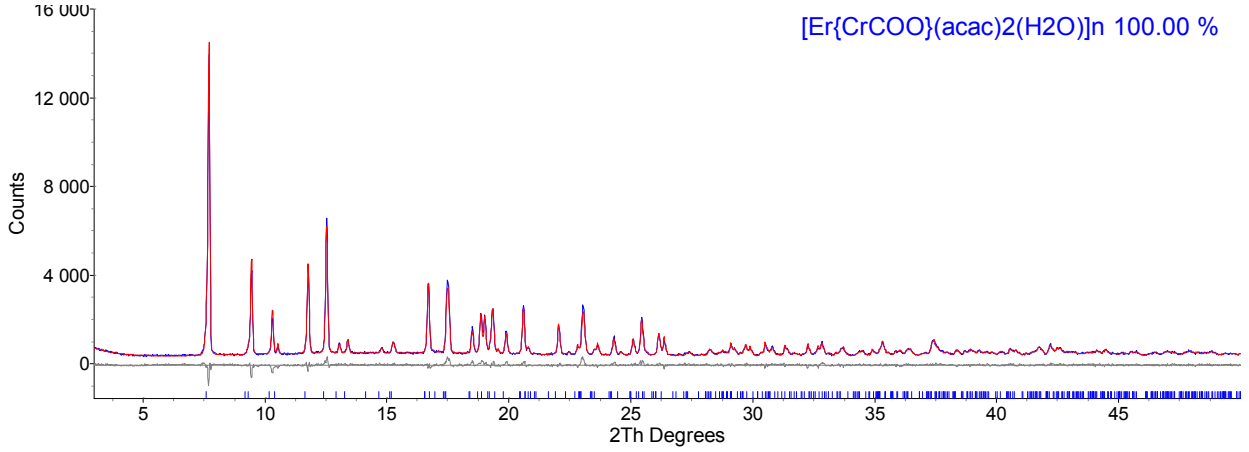
8 000
6 000
4 000
2 000
0
-2 000
5
10
15
20
25
30
35
40
45
50
55
2Th Degrees

b


[Er{CrCOO}(acac)2(H2O)]n 100.00 %
Counts
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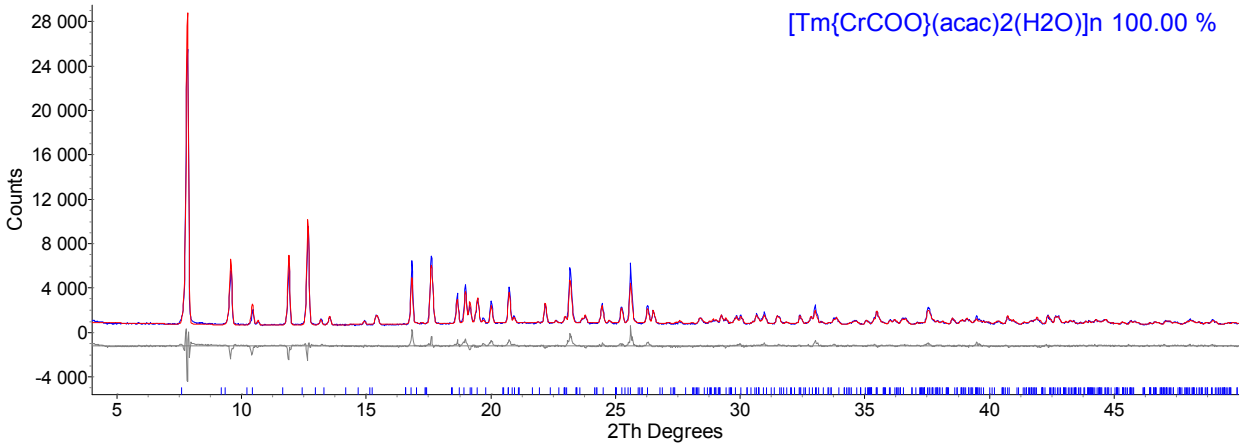
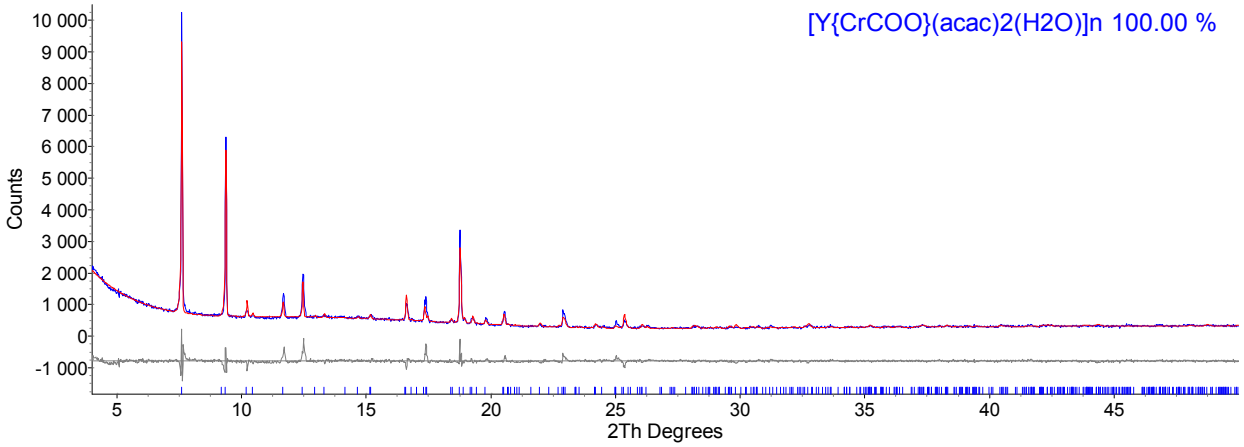
12 000
8 000
4 000
0
5
10
15
20
25
30
35
40
45
2Th Degrees

c



d



e

Fig. S1. Rietveld refinement profiles for (a) **5a**, (b) **3b**, (c) **6**, (d) **7**, and (e) **9** for room temperature X-ray data. The calculated and experimental profiles are shown with the red and blue line, respectively. The bottom trace shows the difference curve. The vertical bars indicate the calculated positions of the Bragg peaks.

Table S3. Hydrogen bonds for **1, 2, 3a** and **4a** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
		1		
O(7)-H(1)...O(3)#1	0.90	1.86	2.750(3)	169
O(7)-H(2B)...O(5)#1	0.90	2.26	3.048(3)	147
O(7)-H(2A)...O(7)#2	0.90	2.16	3.040(4)	167
O(8)-H(3)...O(2)#3	0.90	1.99	2.851(3)	160
O(8)-H(4)...O(5)#3	0.90	1.94	2.794(3)	159
C(4)-H(4A)...O(6)#4	0.95	2.48	3.428(4)	172
C(15)-H(15A)...O(11)#5	0.95	2.74	3.569(4)	146
		2		
O(7)-H(1)...O(3)#1	0.86	1.90	2.747(6)	169
O(7)-H(2B)...O(5)#1	0.89	2.34	3.039(7)	136
O(7)-H(2A)...O(7)#2	0.71	2.35	3.054(9)	168
O(8)-H(3)...O(2)#3	0.74	2.29	2.883(6)	138
O(8)-H(4)...O(5)#3	0.78	2.04	2.796(7)	164
		3a		
O(7)-H(1)...O(3)#1	0.85(4)	1.91(4)	2.750(3)	169(3)
O(7)-H(2B)...O(5)#1	0.88(8)	2.35(7)	3.044(3)	136(6)
O(7)-H(2A)...O(7)#2	0.71(7)	2.36(7)	3.058(4)	168(8)
O(8)-H(3)...O(2)#3	0.73(4)	2.28(4)	2.866(3)	138(4)
O(8)-H(4)...O(5)#3	0.77(4)	2.04(4)	2.795(3)	164(4)
		4a		
O(7)-H(1)...O(3)#1	0.90	1.87	2.755(3)	169
O(7)-H(2A)...O(7)#2	0.90	2.17	3.056(4)	169
O(7)-H(2B)...O(5)#1	0.90	2.40	3.043(3)	128
O(8)-H(3)...O(5)#3	0.90	1.93	2.803(3)	164
O(8)-H(4)...O(2)#3	0.90	2.19	2.868(3)	131

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+1,-z; #2 -x+1,-y+1,-z; #3 x+1,y,z; #4 -x+1,-y+1,-z+1; #5 x,y+1,z

Table S4. Hydrogen bonds for **Eu_1D, 4b, 5b** and **8** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
		Eu_1D		
O(10)-H(1)...O(3)#1	0.77(3)	1.98(3)	2.697(3)	157(3)
O(10)-H(2)...O(5)#1	0.79(3)	2.12(3)	2.813(3)	147(3)
C(15)-H(15A)...O(8)#2	0.95	2.59	3.534(4)	171
		4b		
O(10)-H(1)...O(5)#1	0.92	1.97	2.815(4)	151
O(10)-H(2)...O(3)#1	0.90	1.86	2.697(4)	156
C(15)-H(15A)...O(8)#2	0.95	2.58	3.520(6)	171
		5b		
O(10)-H(1)...O(5)#1	0.94(2)	2.01(2)	2.8149(17)	143.2(17)
O(10)-H(2)...O(3)#1	0.83(2)	1.91(2)	2.6941(17)	157(2)
C(15)-H(15A)...O(8)#2	0.95	2.59	3.537(2)	172
		8		
O(10)-H(1)...O(3)#1	0.89(4)	1.88(4)	2.696(3)	151(4)
O(10)-H(2)...O(5)#1	0.90(4)	2.09(4)	2.815(3)	138(3)
C(15)-H(15A)...O(8)#2	0.95	2.60	3.539(5)	171

Symmetry transformations used to generate equivalent atoms:
#1 -x+1/2,y-1/2,-z+1/2; #2 x-1/2,y+1/2,z

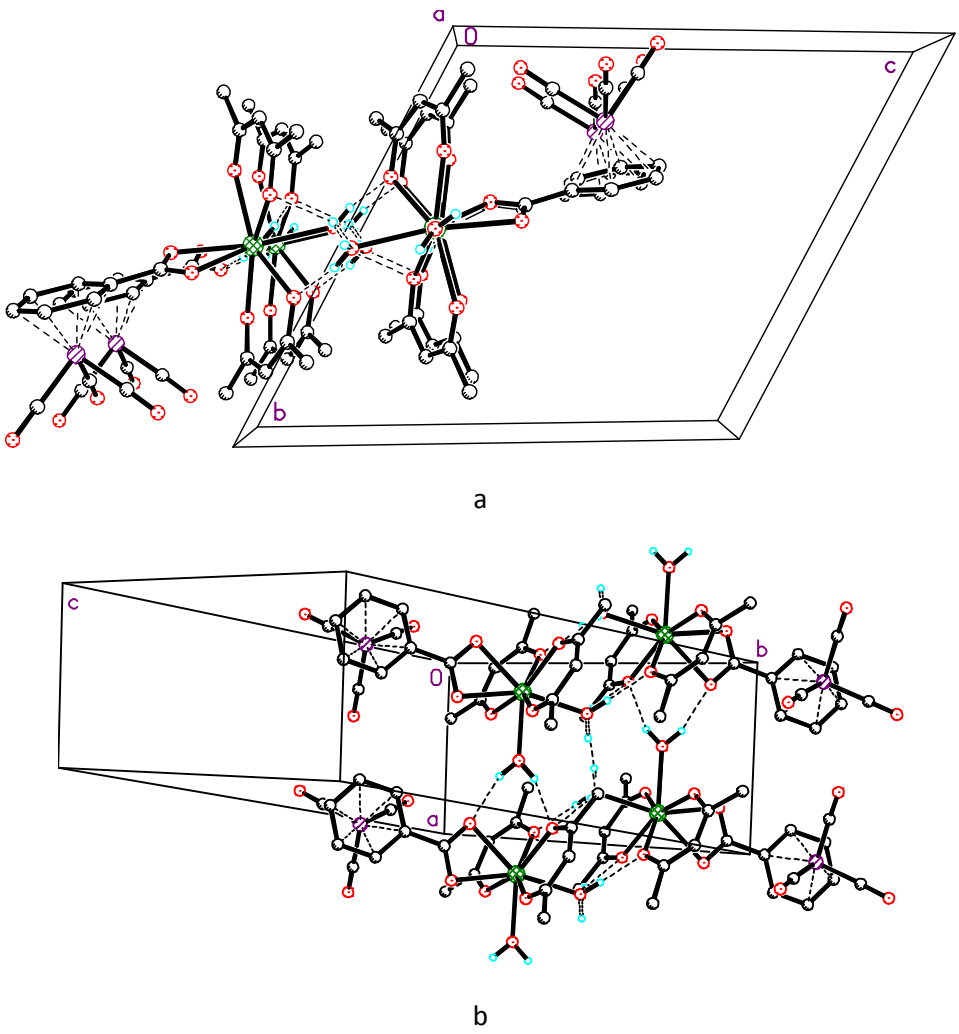


Fig. S2. Fragment of the structure **1**. Projection along [100] (a) and [011] (b).

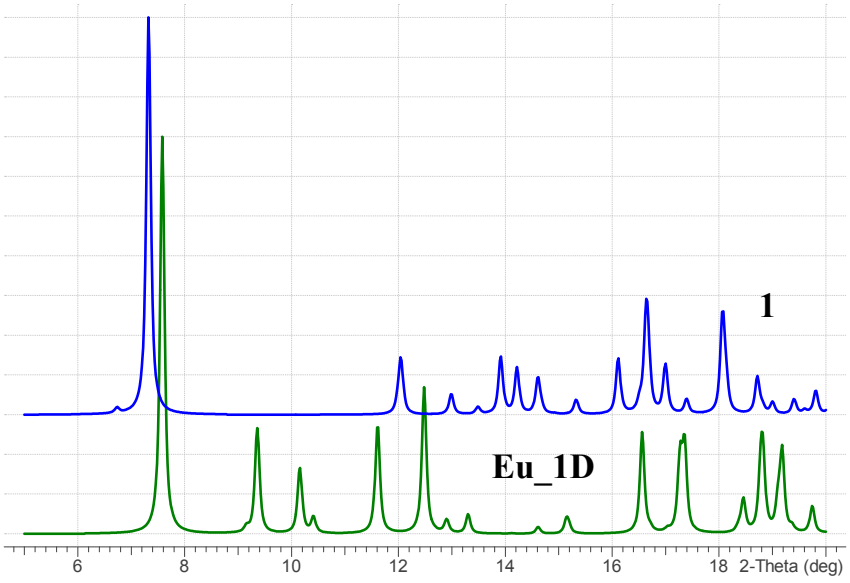


Fig. S3. Calculated X-ray patterns for compounds **1** (blue) and **Eu_1D** (green).

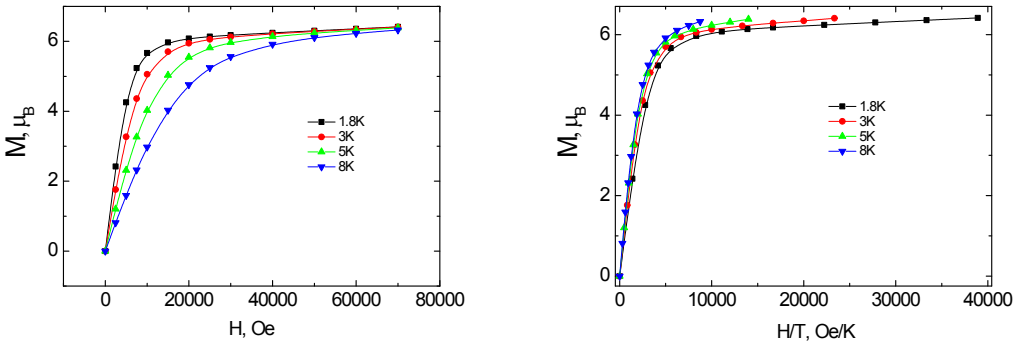


Fig. S4. Field dependences of the magnetization for complex **4a** (Dy) plotted as *M vs. H* (left) and *M vs. H/T* (right) below 8 K. Solid lines are visual guides.

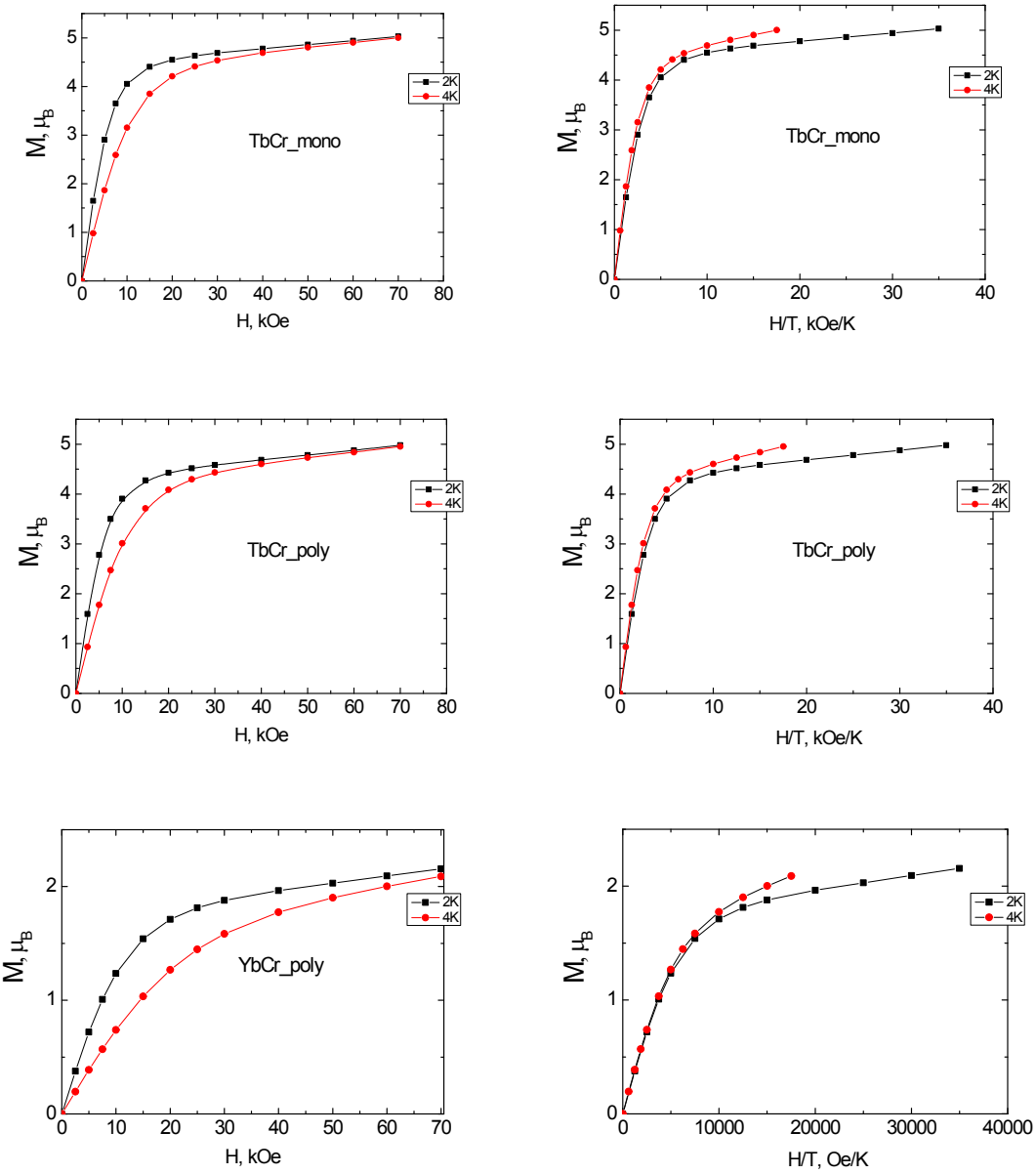


Fig. S5. Field dependences of the magnetization for complexes **3a**, **3b** and **8** (top, middle and bottom parts of the figure respectively) plotted as *M vs. H* (left) and *M vs. H/T* (right) below 4 K. Solid lines are visual guides.

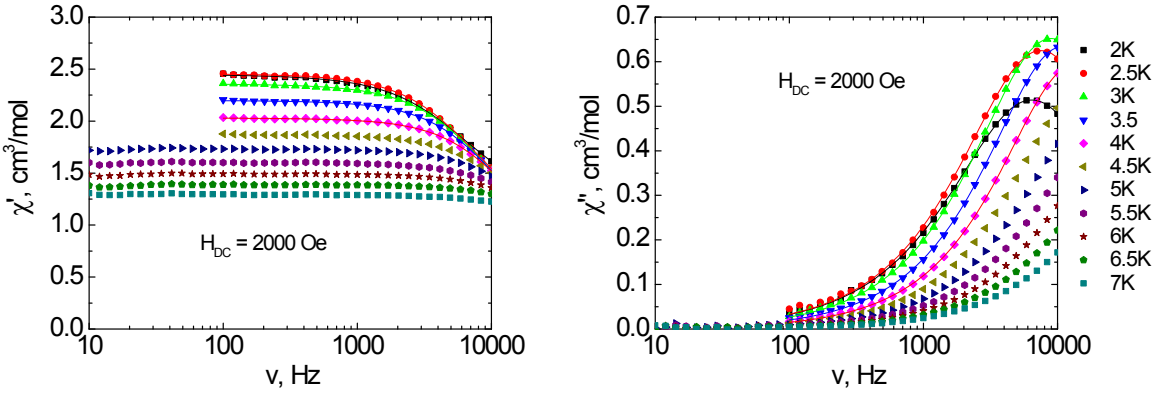


Fig. S6 Frequency dependences of the in-phase χ' (left) and out-of-phase χ″ (right) components of the ac susceptibility of complex **3a** (Tb) in an external magnetic field H = 2000 Oe. Solid lines were fitted using the generalized Debye model.

Table S5. Selected parameters obtained by fitting ac data with the linear combination of two generalized Debye models for **3a** (Tb) in 2000 Oe field.

T (K)	ν (Hz)	Std. Dev.	α	Std. Dev.
2	6407	56	0.128	0.003
2.5	7495	116	0.121	0.005
3	8923	83	0.102	0.003
3.5	10946	122	0.091	0.002
4	13518	167	0.084	0.002

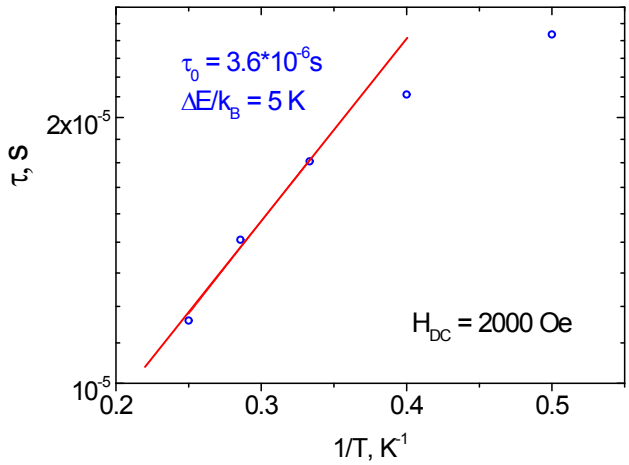


Fig. S7 Dependence of relaxation time on inverse temperature for complex **3a** (Tb) (the relaxation time has been extracted from the frequency dependences of the ac susceptibility shown in Fig. S6). Solid line is the best fit to the Arrhenius law.

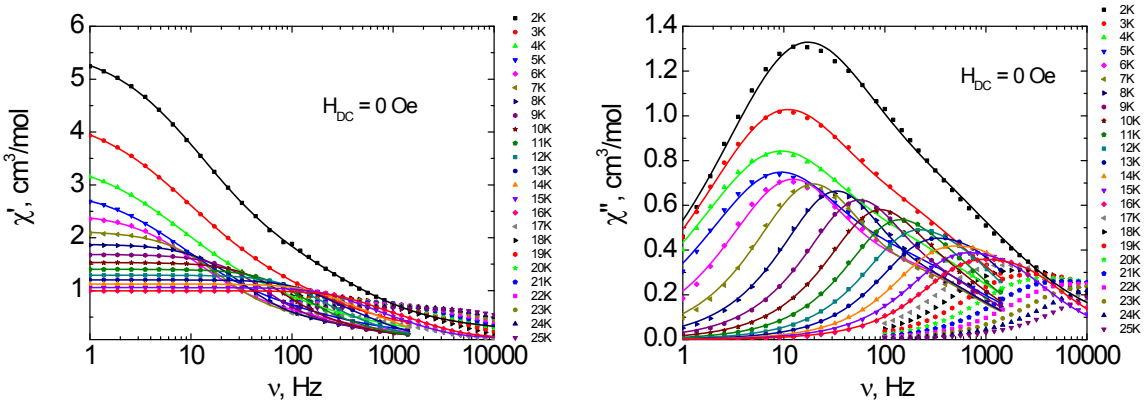


Fig. S8. Frequency dependence of the in-phase χ' (Top left) and out-of-phase χ″ (Bottom right) components of the ac susceptibility of complex **4a** (Dy) in zero dc field. Solid lines were fitted using the linear combination of two generalized Debye models.

Table S6. Selected parameters obtained by fitting ac data with the linear combination of two generalized Debye models for **4a** (Dy) in zero dc field.

T (K)	ν_{HF} (Hz)	Std. Dev.	α	Std. Dev.	ν_{LF} (Hz)	Std. Dev.
2	473	49	0.334	0.011	14.7	0.6
3	250	28	0.306	0.012	9.2	0.4
4	249	31	0.304	0.012	8.1	0.3
5	246	34	0.255	0.015	8.4	0.3
6	267	36	0.172	0.016	11.4	0.4
7	339	42	0.113	0.013	18.6	0.5
8	429	46	0.081	0.010	32	1
9	535	54	0.065	0.008	53	1
10	572	55	0.053	0.008	84	2
11	578	41	0.039	0.008	122	3
12	681	30	0.0227	0.007	169	4
13	848	23	0.009	0.005	221	5
14	1195	39	0.003	0.005	299	6
15	1934	52	0.031	0.007	454	10
16	2665	49	0.025	0.005	598	11

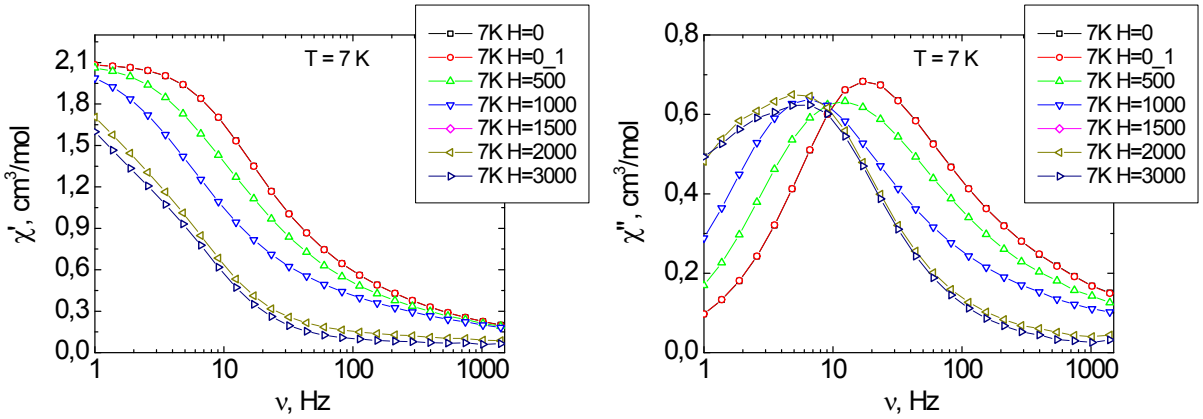


Fig. S9. Frequency dependences of the in-phase χ' (left) and out-of-phase χ″ (right) components of the ac susceptibility of complex **4a** (Dy) in various external magnetic fields 0 - 3000 Oe. Solid lines are visual guides.

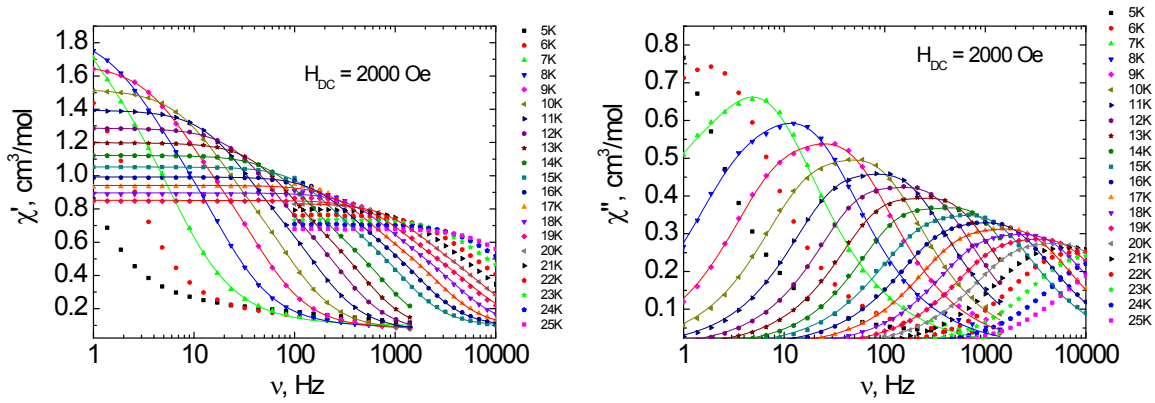
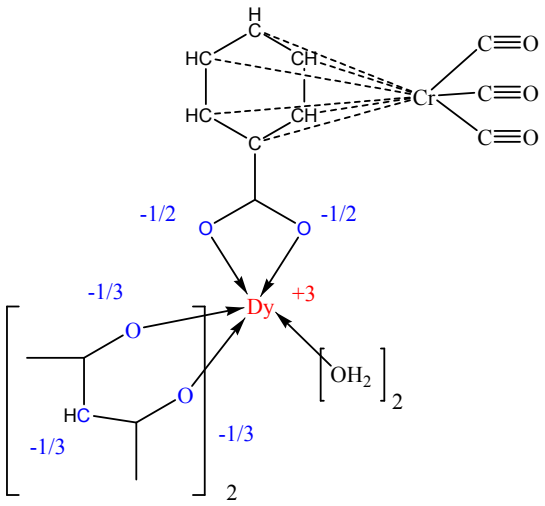


Fig. S10. Frequency dependence of the in-phase χ' (Top left) and out-of-phase χ″ (Bottom right) components of the ac susceptibility of complex **4a** (Dy) in 2000 Oe field. Solid lines were fitted using the linear combination of two generalized Debye models.

Table S7. Selected parameters obtained by fitting ac data with the linear combination of two generalized Debye models for **4a** (Dy) in 2000 Oe field.

T (K)	ν_{HF} (Hz)	Std. Dev.	α	Std. Dev.	ν_{LF} (Hz)	Std. Dev.
7	6.4	0.7	0.164	0.019	0.7	0.4
8	19.7	1.2	0.124	0.015	3.4	0.2
9	47	2	0.089	0.012	7.9	0.3
10	94	3	0.073	0.010	16.1	0.6
11	176	4	0.061	0.007	30	1
12	318	5	0.042	0.006	53	1
13	520	9	0.033	0.006	86	2
14	823	16	0.022	0.006	133	2
15	1263	22	0.061	0.006	220	4
16	1945	25	0.054	0.005	342	5
17	2943	31	0.043	0.004	525	6
18	4328	43	0.037	0.004	792	9
19	6240	70	0.031	0.003	1186	13
20	8885	163	0.027	0.003	1775	24



Scheme S1. Partial charges assigned to complex **4a**.

Output file of MAGELLAN program assuming charges acording to Sceme S1:

Site	Optimized energy (cm-1)	Curvature eigenvalues		Min. reversal energy (cm-1)
1	-0.2113E+03	0.7064E+03	0.2173E+03	0.2165E+03

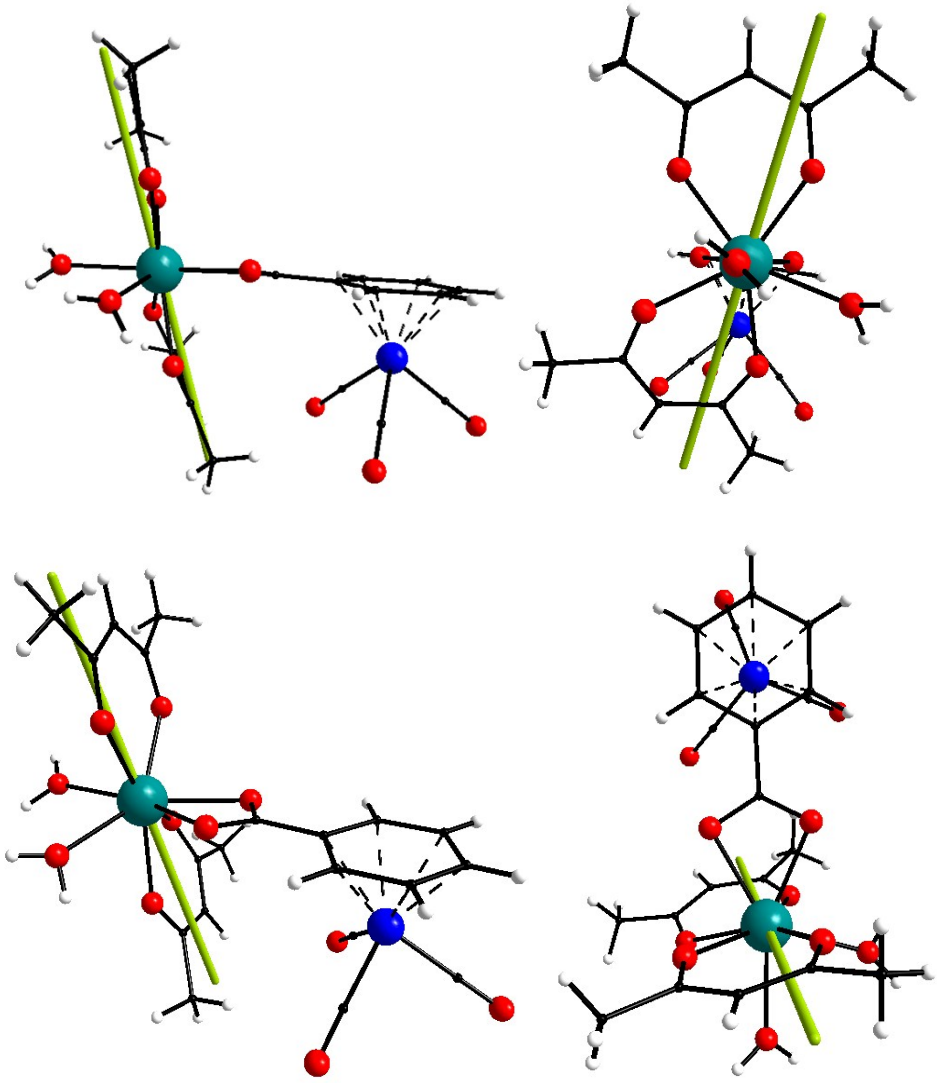
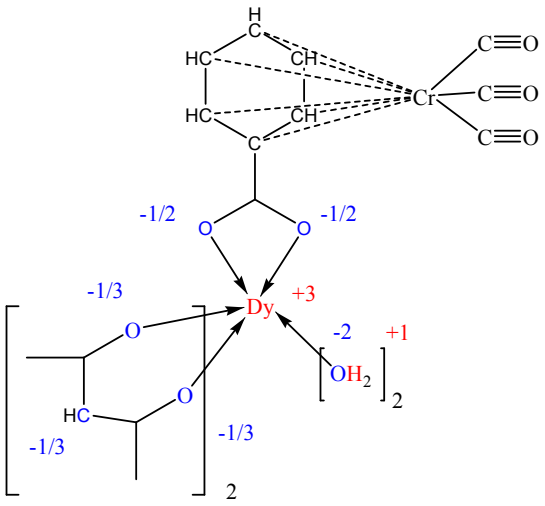


Fig. S11. Calculated magnetic anisotropy axes in **4a** assuming charges acording to Sceme S1.



Scheme S2. Partial charges assigned to complex **4a**.

Output file of MAGELLAN program assuming charges acording to Sceme S2 with the H2A position of the water hydrogen:

Site	Optimized energy (cm-1)	Curvature eigenvalues		Min. reversal energy (cm-1)
1	-0.5454E+03	0.2247E+04	0.1006E+04	0.9923E+03

Output file of MAGELLAN program assuming charges acording to Sceme S2 with the H2B position of the water hydrogen:

Site	Optimized energy (cm-1)	Curvature eigenvalues		Min. reversal energy (cm-1)
1	-0.4399E+03	0.2003E+04	0.6786E+03	0.7785E+03

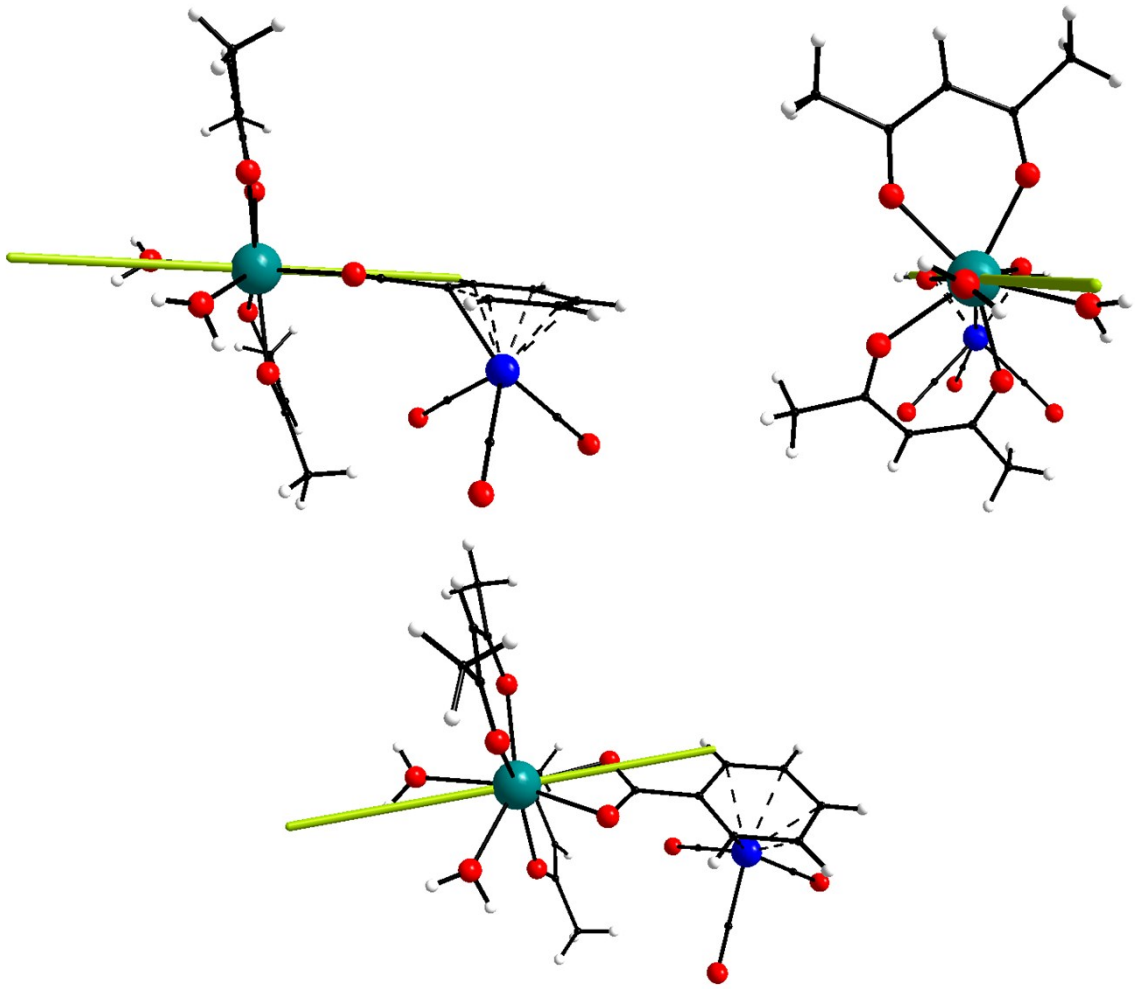
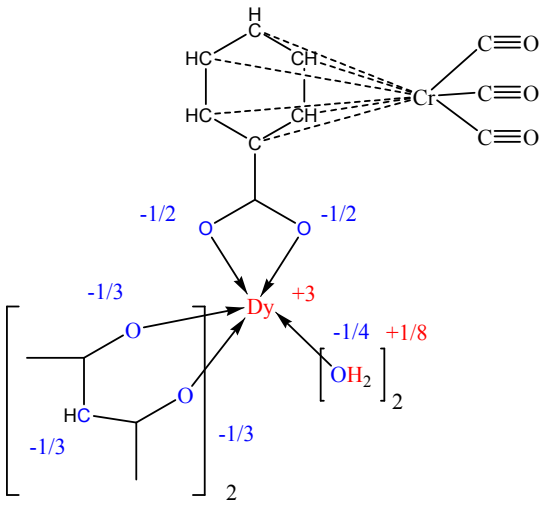


Fig. S12. Calculated magnetic anisotropy axes in **4a** assuming charges acording to Sceme S2 (with the H2A position of the water hydrogen).



Scheme S3. Partial charges assigned to complex **4a**.

Output file of MAGELLAN program assuming charges acording to Sceme S3 with the H2A position of the water hydrogen:

Site	Optimized energy (cm-1)	Curvature eigenvalues		Min. reversal energy (cm-1)
1	-0.1488E+03	0.4591E+03	0.2003E+03	0.1499E+03

Output file of MAGELLAN program assuming charges acording to Sceme S3 with the H2B position of the water hydrogen:

Site	Optimized energy (cm-1)	Curvature eigenvalues		Min. reversal energy (cm-1)
1	-0.1586E+03	0.4664E+03	0.2347E+03	0.1861E+03

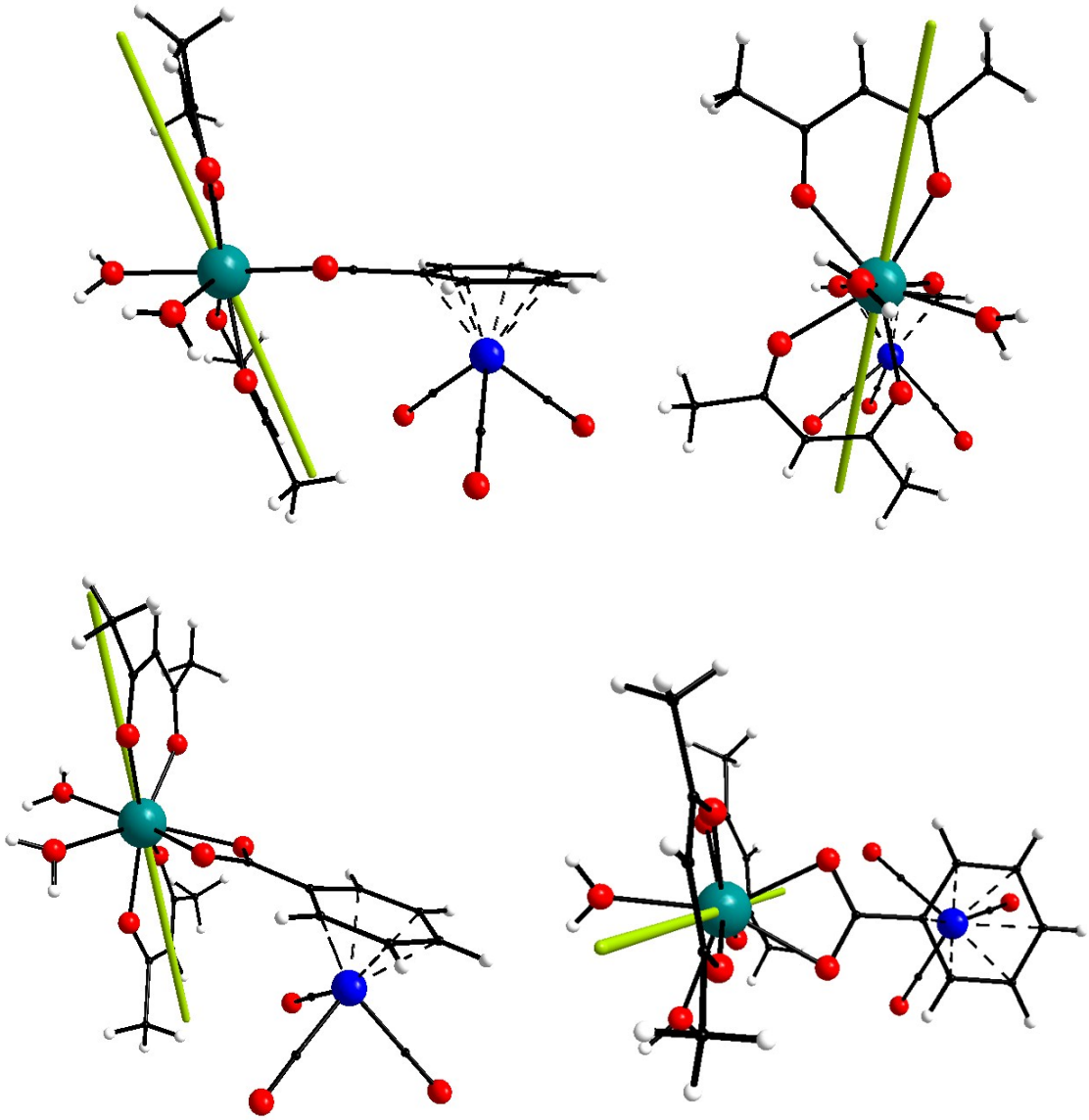


Fig. S13. Calculated magnetic anisotropy axes in **4a** assuming charges acording to Sceme S3 (with the H2A position of the water hydrogen).

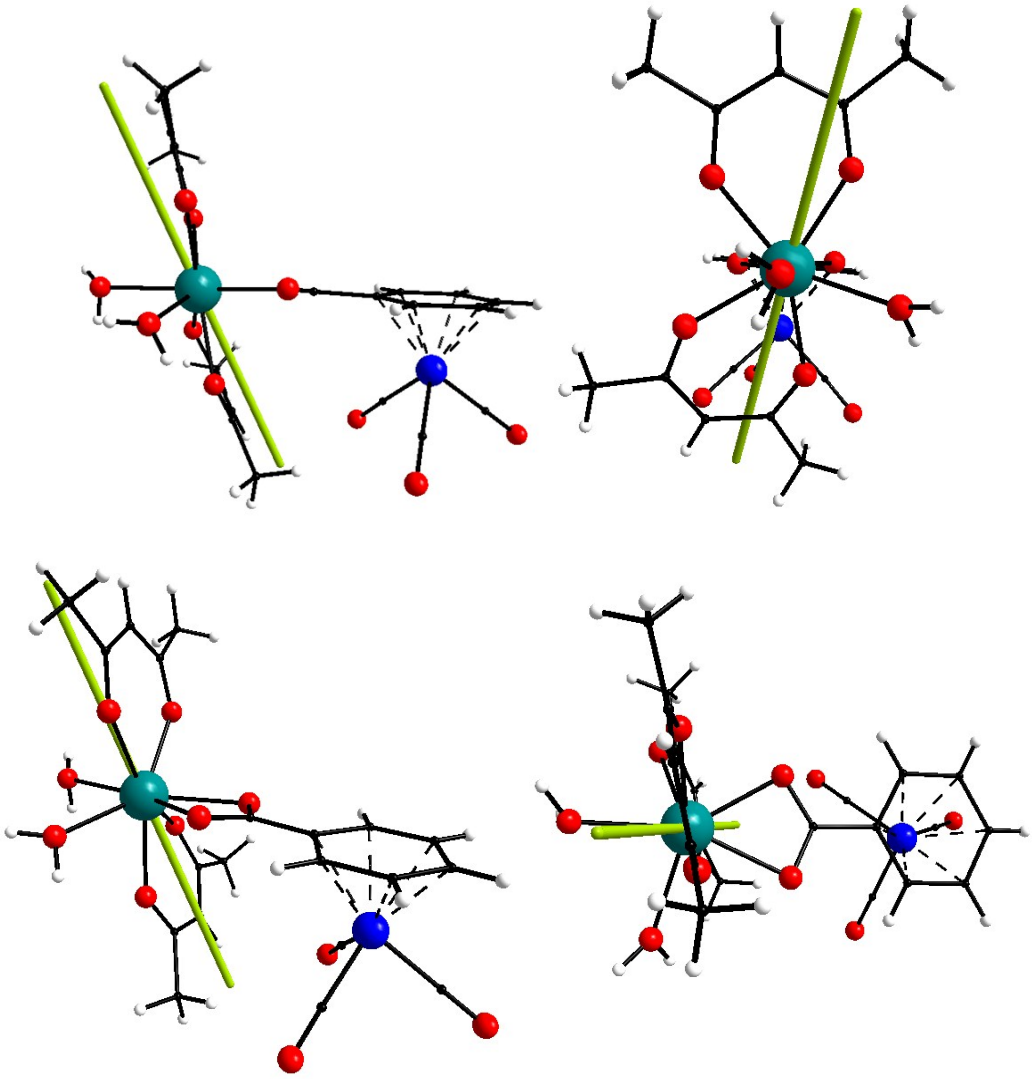


Fig. S14. Calculated magnetic anisotropy axes in **4a** assuming charges acording to Sceme S3 (with the H2B position of the water hydrogen).

Input file for MAGELLAN program for Dy_Bcr_mono (**4a**) (Scheme S3 for taking in consideration H2A position of the water hydrogen):

```
!sites 1 1
Dy    0.00000   0.00000   0.00000   3
Cr    1.05274  -5.80690   0.54925   0
O    -0.58440  -2.03893   1.16021  -0.5
O     1.54595  -1.76351   0.59339  -0.5
O     1.68570   0.13125  -1.64021  -0.33
O    -0.63072  -1.40008  -1.69042  -0.33
O     1.65145   1.27234   1.08820  -0.33
O    -0.92631   0.80548   1.97239  -0.33
O    -0.37888   2.17869  -0.97891  -0.25
H     0.16545   2.89525  -0.96244   0.125
H    -1.09118   2.40458  -1.48057   0.125
O    -2.36571   0.09841  -0.40358  -0.25
H    -3.06372   0.66377  -0.45954   0.125
H    -2.74320  -0.64941  -0.73267   0.125
O    -1.33137  -6.40521  -1.16922   0
O     2.36245  -4.82494  -1.96441   0
O     2.09606  -8.50868  -0.21055   0
C     0.59907  -2.47476   1.07629   0
C     0.90730  -3.84572   1.58762   0
C    -0.15469  -4.66414   2.02096   0
H    -1.04909  -4.35332   1.94394   0
C     0.09718  -5.94654   2.57073   0
H    -0.61994  -6.48587   2.88275   0
C     1.42363  -6.40960   2.64796   0
H     1.59861  -7.27647   2.99498   0
C     2.49885  -5.60050   2.21549   0
H     3.39193  -5.91565   2.29030   0
C     2.24340  -4.32713   1.67388   0
H     2.96304  -3.78890   1.36580   0
C     3.45731  -0.56258  -3.05816   0
H     3.60594  -1.20353  -3.78444   0
H     4.10774  -0.72284  -2.34284   0
H     3.56578   0.34943  -3.40001   0
C     2.06649  -0.73240  -2.51739   0
C     1.29501  -1.78871  -2.98145  -0.33
H     1.68212  -2.36444  -3.63043   0
C    -0.01093  -2.06814  -2.56390   0
C    -0.75144  -3.23025  -3.17869   0
H    -0.40018  -3.40293  -4.07714   0
H    -1.70586  -3.01551  -3.23679   0
H    -0.62923  -4.02709  -2.62144   0
C     2.92180   2.90952   2.23874   0
H     2.88625   3.40004   3.08639   0
H     3.00381   3.54468   1.49695   0
H     3.69590   2.30856   2.24130   0
C     1.66411   2.10527   2.07253   0
C     0.61839   2.28835   2.96007  -0.33
H     0.74219   2.91253   3.66546   0
C    -0.61223   1.61702   2.89172   0
C    -1.62291   1.86149   3.98379   0
H    -1.62370   2.81230   4.22127   0
H    -1.38794   1.32820   4.77169   0
H    -2.51391   1.60289   3.66814   0
C    -0.43235  -6.15812  -0.48608   0
C     1.85793  -5.17781  -0.99381   0
C     1.68646  -7.47538   0.08445   0
```

Input file for MAGELLAN program for Dy_Bcr_mono (**4a**) (Scheme S3 for taking in consideration H2B position of the water hydrogen):

```
!sites 1 1
Dy     0.00000   0.00000   0.00000   3
Cr     1.05274  -5.80690   0.54925   0
O     -0.58440  -2.03893   1.16021  -0.5
O      1.54595  -1.76351   0.59339  -0.5
O      1.68570   0.13125  -1.64021  -0.33
O     -0.63072  -1.40008  -1.69042  -0.33
O      1.65145   1.27234   1.08820  -0.33
O     -0.92631   0.80548   1.97239  -0.33
O     -0.37888   2.17869  -0.97891  -0.25
H      0.16545   2.89525  -0.96244   0.125
H     -0.18369   2.00654  -1.84053   0.125
O     -2.36571   0.09841  -0.40358  -0.25
H     -3.06372   0.66377  -0.45954   0.125
H     -2.74320  -0.64941  -0.73267   0.125
O     -1.33137  -6.40521  -1.16922   0
O      2.36245  -4.82494  -1.96441   0
O      2.09606  -8.50868  -0.21055   0
C      0.59907  -2.47476   1.07629   0
C      0.90730  -3.84572   1.58762   0
C     -0.15469  -4.66414   2.02096   0
H     -1.04909  -4.35332   1.94394   0
C      0.09718  -5.94654   2.57073   0
H     -0.61994  -6.48587   2.88275   0
C      1.42363  -6.40960   2.64796   0
H      1.59861  -7.27647   2.99498   0
C      2.49885  -5.60050   2.21549   0
H      3.39193  -5.91565   2.29030   0
C      2.24340  -4.32713   1.67388   0
H      2.96304  -3.78890   1.36580   0
C      3.45731  -0.56258  -3.05816   0
H      3.60594  -1.20353  -3.78444   0
H      4.10774  -0.72284  -2.34284   0
H      3.56578   0.34943  -3.40001   0
C      2.06649  -0.73240  -2.51739   0
C      1.29501  -1.78871  -2.98145  -0.33
H      1.68212  -2.36444  -3.63043   0
C     -0.01093  -2.06814  -2.56390   0
C     -0.75144  -3.23025  -3.17869   0
H     -0.40018  -3.40293  -4.07714   0
H     -1.70586  -3.01551  -3.23679   0
H     -0.62923  -4.02709  -2.62144   0
C      2.92180   2.90952   2.23874   0
H      2.88625   3.40004   3.08639   0
H      3.00381   3.54468   1.49695   0
H      3.69590   2.30856   2.24130   0
C      1.66411   2.10527   2.07253   0
C      0.61839   2.28835   2.96007  -0.33
H      0.74219   2.91253   3.66546   0
C     -0.61223   1.61702   2.89172   0
C     -1.62291   1.86149   3.98379   0
H     -1.62370   2.81230   4.22127   0
H     -1.38794   1.32820   4.77169   0
H     -2.51391   1.60289   3.66814   0
C     -0.43235  -6.15812  -0.48608   0
C      1.85793  -5.17781  -0.99381   0
C      1.68646  -7.47538   0.08445   0
```

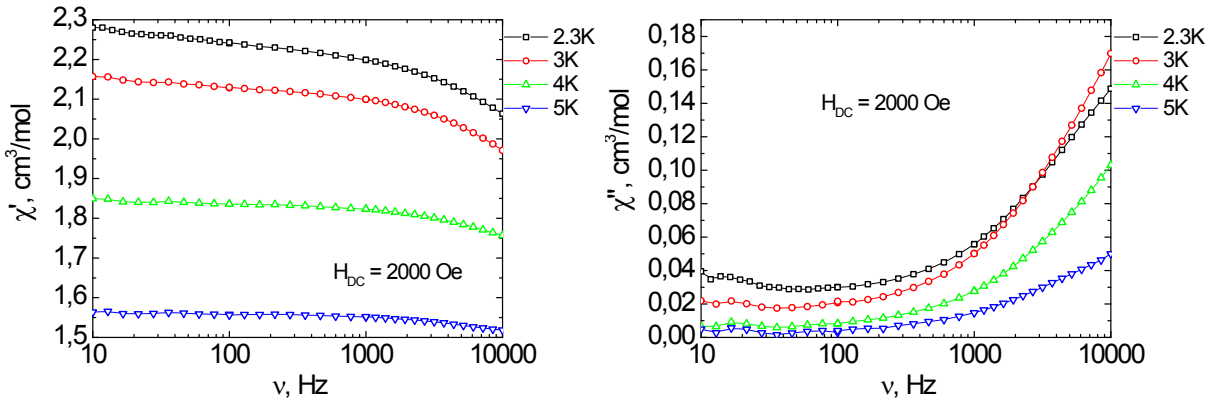


Fig. S15. Frequency dependences of the in-phase χ' (left) and out-of-phase χ″ (right) components of the ac susceptibility of complex **3b** (Tb) in 2000 Oe dc-field. Solid lines are visual guides.

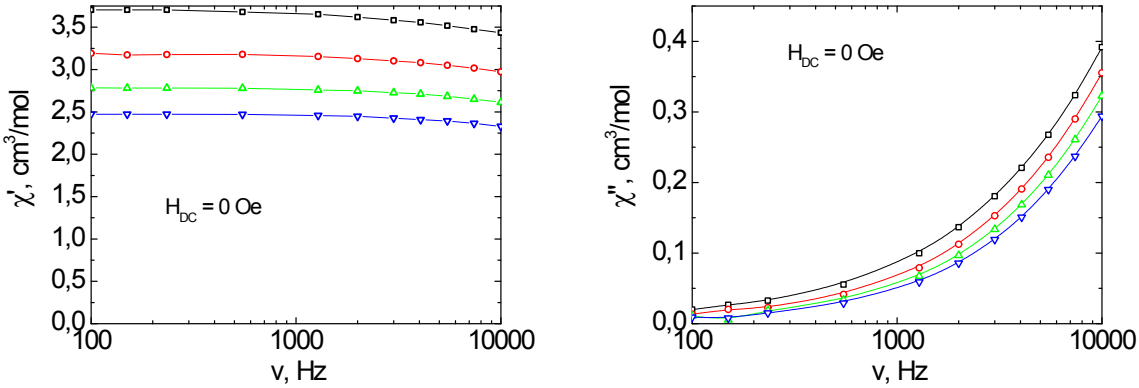


Fig. S16. Frequency dependences of the in-phase χ' (left) and out-of-phase χ″ (right) components of the ac susceptibility of complex **4b** (Dy) in zero magnetic field. Solid lines are visual guides.

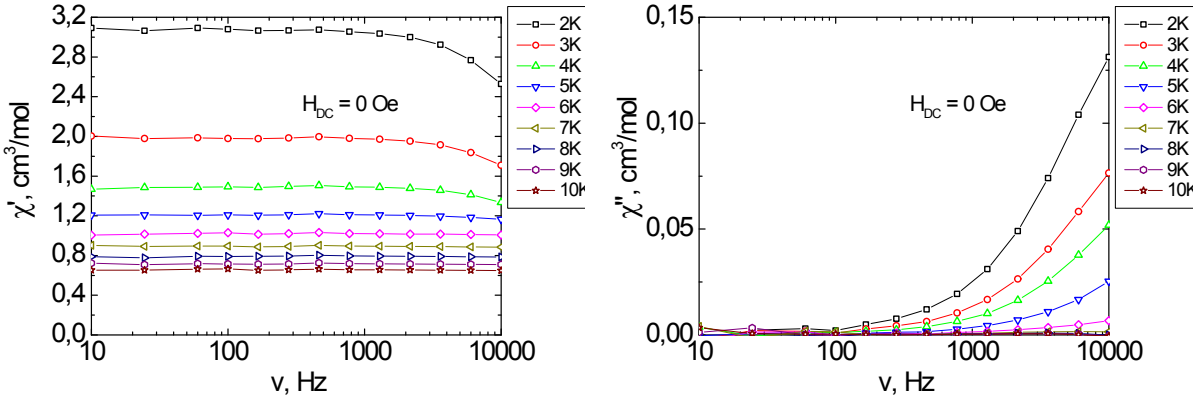


Fig. S17. Frequency dependences of the in-phase χ' (left) and out-of-phase χ″ (right) components of the ac susceptibility of complex **6** (Er) in zero magnetic field. Solid lines are visual guides.

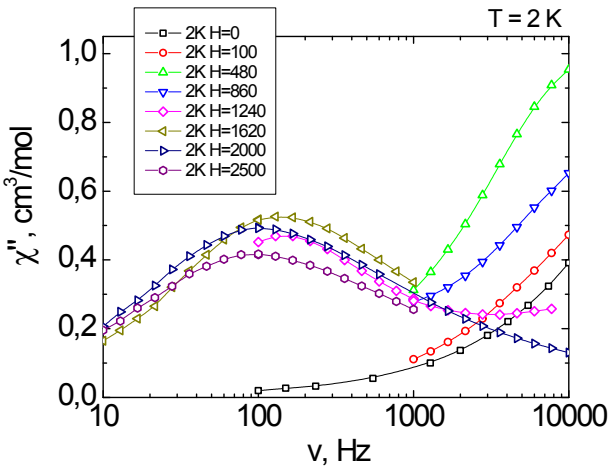


Fig. S18. Frequency dependences of the i out-of-phase χ″ components of the ac susceptibility of complex **4b** (Dy) in various external magnetic fields 0 - 2500 Oe. Solid lines are visual guides

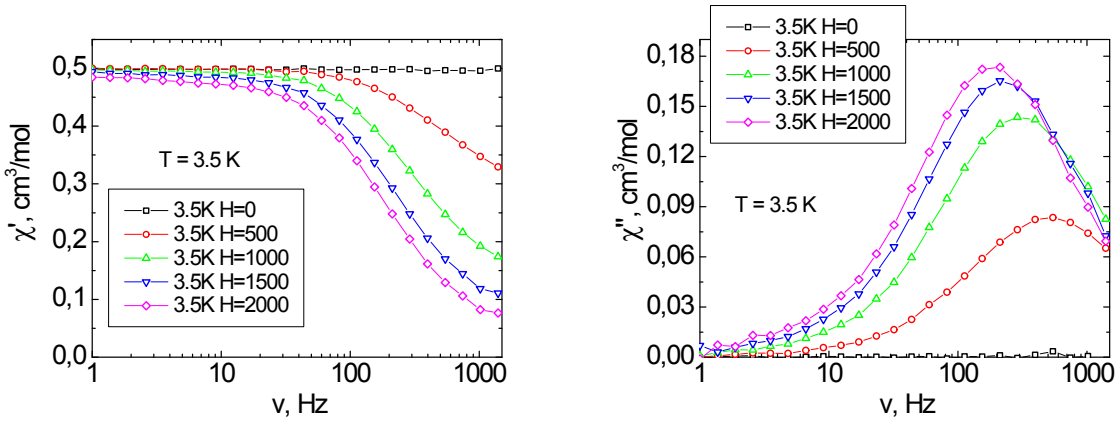


Fig. S19. Frequency dependences of the in-phase χ' (left) and out-of-phase χ″ (right) components of the ac susceptibility of complex **8** (Yb) in various external magnetic fields 0 - 2000 Oe. Solid lines are visual guides.

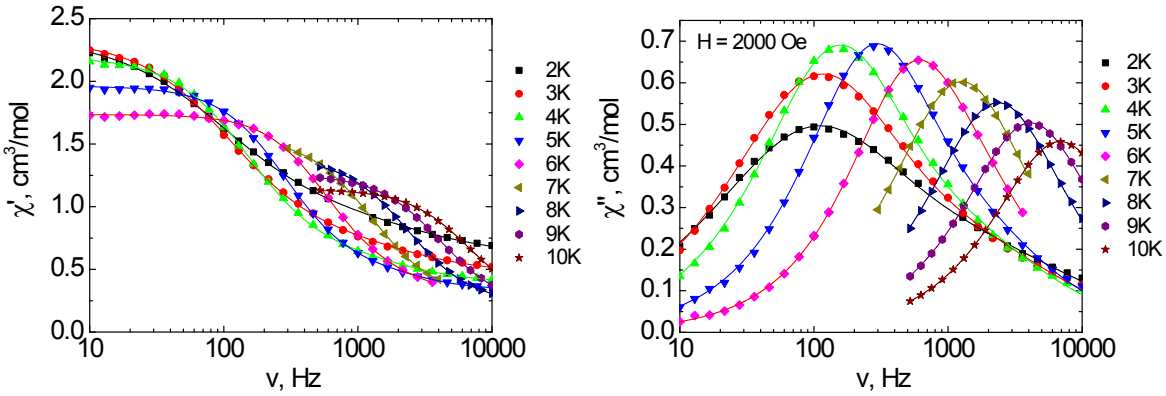


Fig. S20. Frequency dependences of the in-phase χ' (left) and out-of-phase χ″ (right) components of the ac susceptibility of complex **4b** (Dy) in an external magnetic field H = 2000 Oe. Solid lines were fitted using the linear combination of two generalized Debye models.

Table S8. Selected parameters obtained by fitting ac data with the linear combination of two generalized Debye models **4b** (Dy) in 2000 Oe field.

T (K)	ν_{HF} (Hz)	Std. Dev.	α	Std. Dev.	ν_{LF} (Hz)	Std. Dev.
2	2786	369	0.278	0.008	101	2
3	2346	303	0.202	0.008	111	2
4	2213	243	0.115	0.007	152	2
5	2688	263	0.060	0.006	286	4
6	2264	227	0.025	0.003	570	9
7			0.049	0.004	1265	5
8			0.040	0.003	2362	8
9			0.026	0.002	4127	10
10			0.021	0.001	6858	17

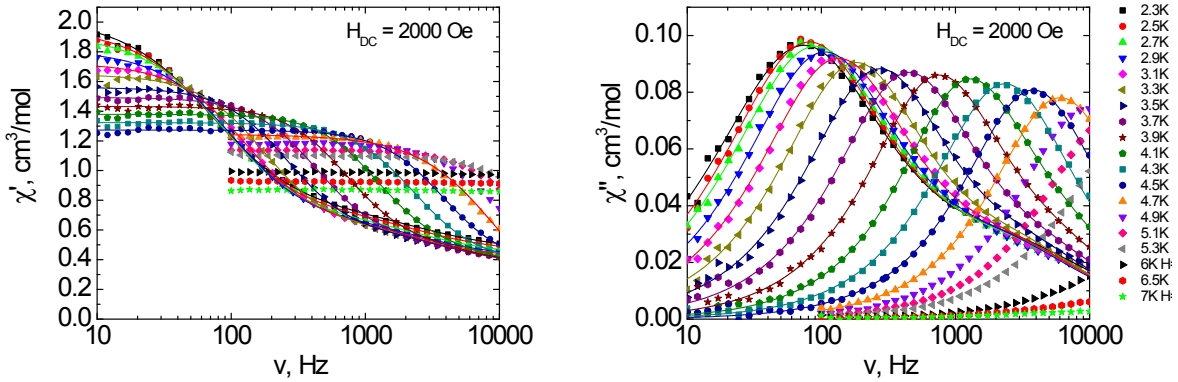


Fig. S21. Frequency dependences of the in-phase χ' (left) and out-of-phase χ″ (right) components of the ac susceptibility of complex **6** (Er) in an external magnetic field 2000 Oe. Solid lines were fitted using the linear combination of two generalized Debye models.

Table S9. Selected parameters obtained by fitting ac data with the linear combination of two generalized Debye models for **6** (Er) in 2000 Oe field.

T (K)	ν_{HF} (Hz)	Std. Dev.	α	Std. Dev.	ν_{LF} (Hz)	Std. Dev.
2.3	3055	330	0.179	0.008	72	1
2.5	2768	245	0.148	0.008	79	1
2.7	2945	234	0.145	0.006	87	1
2.9	2797	252	0.119	0.008	103	1
3.1	3043	248	0.105	0.007	130	2
3.3	3302	306	0.083	0.007	176	3
3.5	4123	460	0.077	0.007	265	4
3.7	5507	1030	0.069	0.009	436	9
3.9	6386	1771	0.048	0.011	728	21
4.1	7162	3001	0.030	0.014	1228	57
4.3	-	-	0.057	0.004	2332	16
4.5	-	-	0.044	0.006	3798	37
4.7	-	-	0.030	0.002	9377	69

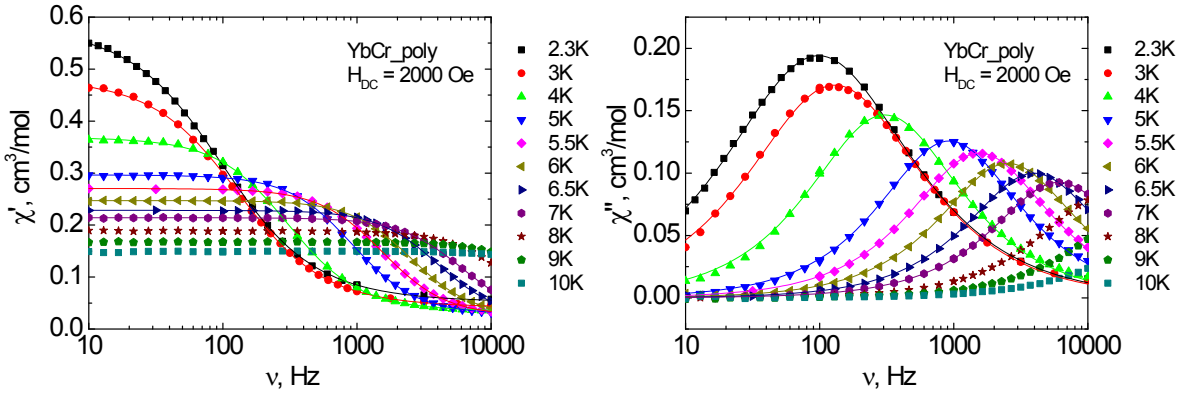


Fig. S22. Frequency dependences of the in-phase χ' (left) and out-of-phase χ″ (right) components of the ac susceptibility of complex **8** (Yb) in an external magnetic field 2000 Oe. Solid lines were fitted using the generalized Debye model.

Table S10. Selected parameters obtained by fitting ac data with the generalized Debye model for **8** (Yb) in 2000 Oe field.

T (K)	ν (Hz)	Std. Dev.	α	Std. Dev.
2.3	98	1	0.196	0.003
3	130	1	0.161	0.004
4	307	2	0.090	0.005
5	926	5	0.047	0.003
5.5	1557	5	0.039	0.002
6	2531	9	0.031	0.003
6.5	3976	17	0.023	0.003
7	6072	25	0.020	0.002

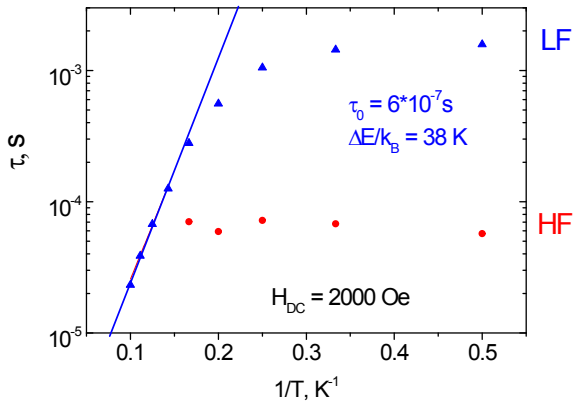


Fig. S23. Dependence of relaxation time on inverse temperature for complex **4b** (Dy) (the points are based on data of frequency dependences of ac susceptibility in an external magnetic field H = 2000 Oe). Solid line is the best fit to the Arrhenius law.

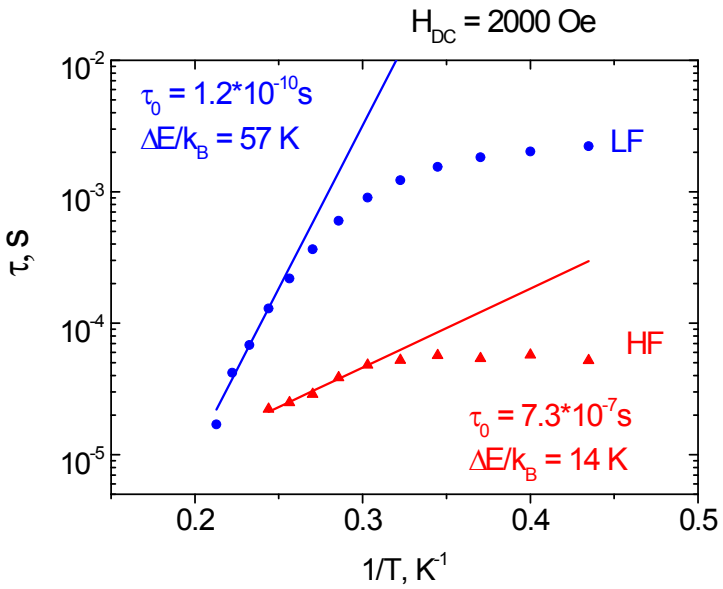


Fig. S24. Dependence of relaxation time on inverse temperature for complex **6** (Er) (the points are based on data of frequency dependences of ac susceptibility in an external magnetic field H = 2000 Oe). Solid line is the best fit to the Arrhenius law.

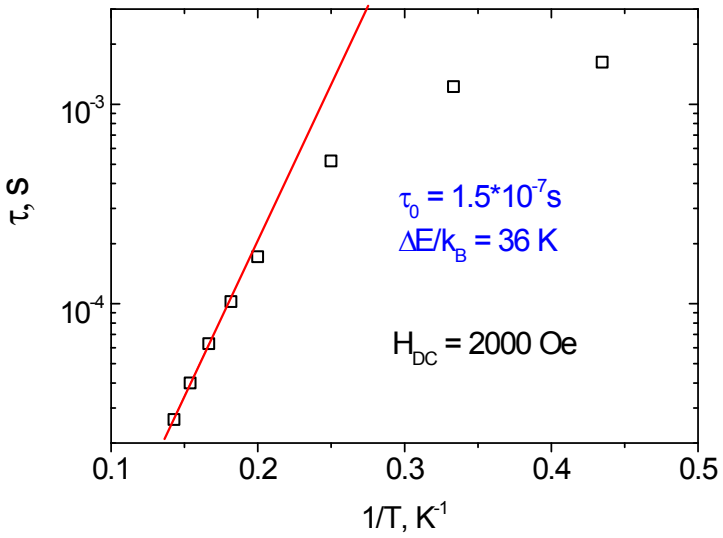


Fig. S25. Dependence of relaxation time on inverse temperature for complex **8** (Yb) (the points are based on data of frequency dependences of ac susceptibility in an external magnetic field H = 2000 Oe). Solid line is the best fit to the Arrhenius law.